

Contemporary
Concepts
in Physics
Volume 9

Marcos Moshinsky
and
Yuri F. Smirnov

**The Harmonic
Oscillator in
Modern
Physics**

Contemporary Concepts in Physics

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The Harmonic Oscillator in Modern Physics

Marcos Moshinsky

and

Yuri F. Smirnov

Instituto de Física
Universidad Nacional Autónoma de México



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A Esperanza y a la memoria de Elena y de mis padres
— Marcos

To Rita and the memory of my parents
— Yuri

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Preface to the Series

The series of volumes, *Contemporary Concepts in Physics*, is addressed to the professional physicist and to the serious graduate student of physics. The subjects to be covered will include those at the forefront of current research. It is anticipated that the various volumes in the series will be rigorous and complete in their treatment, supplying the intellectual tools necessary for the appreciation of the present status of the areas under consideration and providing the framework upon which future developments may be based.

Preface

The harmonic oscillator has been a basic tool in physics for many centuries. It is said, for example, that Galileo checked the constancy of the period of the small oscillations of a pendulum by comparing them with his heartbeat; it would not be surprising if even Archimedes were aware of some of the properties of these types of motion.

The full importance of the harmonic oscillator as a basic tool for the development of theoretical physics probably became apparent with the birth of quantum mechanics. It was the first example to which quantization rules were applied, and since then its spectra, wave functions, symmetries, and so on, have had innumerable applications not only in direct calculations, but also as a model to increase our understanding of more complex problems.

Professor Moshinsky wrote a slim volume in 1969 with a title similar to the present work. It required as background a course in standard quantum mechanics and knowledge of angular momentum theory, which is now called Racah algebra. This early version was intended to give a glimpse of the many applications of the harmonic oscillator one could learn starting from limited knowledge. Dr. Smirnov, in addition to his contributions to the application of harmonic oscillators in many fields of physics, translated the original version into Russian and thus was thoroughly familiar with its contents.

In 1993 Dr. Smirnov came to the Instituto de Física of the Universidad Nacional Autónoma de México (U.N.A.M.), and, working together, the two authors enlarged the original book to include many more applications — particularly to scattering problems, collective motion in nuclei, and relativistic examples. Necessary background also required a course in group theory, though most of the latter material appears, *ab initio*, in chapter VII of this volume.

Professor Moshinsky would like to express his gratitude to El Colegio Nacional for the support he has received from this institution through the years and, in particular, for its help in consolidation of the material of the present publication. Both authors are also indebted to Consejo Nacional de Ciencia y

Tecnología in Mexico for support through the Sistema Nacional de Investigadores and the Cátedras Patrimoniales.

We would like to thank those who aided us in the preparation of this book: Dr. Elpidio Chacón, who revised many of the chapters and modernized some of the notation; Drs. Peter O. Hess and Alejandro Frank, who revised chapters IX and X of the book, respectively, and provided some of the figures and results of calculations; Professors Gennady F. Filippov, Peter Kramer, and Christiane Quesne, in collaboration with whom material of different parts of the volume was developed. Then graduate students A. Del Sol Mesa, A. García Zenteno, and G. Loyola collaborated in the research of some of the chapters and also revised parts of the book. Tatiana Nevskaya helped with some of the computations; Beatriz Aizen typed the first version of the manuscript; and Fanny Arenas helped greatly in transferring the manuscript to diskette.

We are indebted to so many colleagues in Mexico, Russia, and other countries for helpful discussions that we risk omitting some if we attempt to name them all. To all those who may recognize our conversations in some parts of the book, we wish to say simply: Thank you.

Introduction

Our objective in this Introduction is to give a brief outline of the main parts of this book and to indicate the background knowledge required to understand each, as well as how to use the book more effectively.

This book has 13 chapters with 70 sections, and is divided essentially into five parts.

The first part (chapters I to V) deals with applications of many body states with oscillator interactions, starting with one and ending with four particles, where the analysis is complete, and continuing with n particles but only in the Hartree-Fock approximation.

To understand these first five chapters, a standard course in quantum mechanics combined with ample knowledge of angular momentum theory is required. For the latter, the usual Clebsch-Gordan and Racah coefficients of the rotation group have been put in the $3j$ and $6j$ form, at present more familiar notations, though occasionally this adds a few phase factors to the formulas. For the permutation group, the analysis is self-contained except for Eq. (17.15) which is derived in standard books of group theory, though it also could be accepted as the basis for Eqs. (17.16–18) and the reasoning continues to be self-contained from there.

The second part of the book (chapter VI) deals with the application of harmonic oscillator states to scattering problems where, at first glance, one would think they play no role, as they vanish at infinity. Approximate phase shifts for potential scattering are obtained explicitly, as well as variational procedures for using harmonic oscillator states in determining resonant levels. A standard knowledge of scattering theory given in a quantum mechanics course is required.

In the third part (chapter VII), a serious attempt is made to understand the group theory underlying the harmonic oscillator, starting with the simple case of the oscillator for one particle in one dimension and ending with m particles in n dimensions. The particular case of interest when $n = 3$ is discussed with reference to some applications to nuclear structure in the 2s–1d shell. We tried to make the analysis completely self-contained.

The fourth part (chapters VIII, IX, and X) deals respectively with four-, five-, and six-dimensional oscillators and their application to the Coulomb problem, the Bohr-Mottelson collective nuclear model, and the Interacting Boson Model (IBM). All that is required for their understanding is presented in previous sections — in particular chapter VII, with the exception of section 42 where some more advanced group theoretical notions are needed.

Finally, the fifth part (chapters XI, XII, and XIII) deals with the relativistic many body problems with oscillator interactions, though the discussion is mainly restricted to systems of one, two, and three particles and applied to the mass spectra of mesons (quark-antiquark systems) and baryons (three quark systems). Knowledge of the elements of the special theory of relativity and, in quantum mechanics, of the Dirac and Klein-Gordon equations, is assumed, though otherwise this part is again self-contained.

In the Conclusions we stress that we have touched only on some aspects of the harmonic oscillator in modern physics related to our own work, or to that of those with whom we have come in personal contact.

Chapter I

The One-Body Problem

1 The Radial Wave Function of the Harmonic Oscillator

We begin by recalling some results that may be found in any elementary quantum-mechanics text. The time-independent Schrödinger equation for the harmonic oscillator in units in which, \hbar, m and the frequency of the oscillator are equal to 1 becomes

$$(-\frac{1}{2}\nabla^2 + \frac{1}{2}r^2)\psi = E\psi. \quad (1.1)$$

Assuming a solution of the form

$$\psi = \frac{\phi(r)}{r} e^{-\frac{1}{2}r^2} Y_{lm}(\vartheta, \varphi) \equiv \psi_{nlm}(\mathbf{x}) = \langle \mathbf{x} | nlm \rangle \equiv | nlm \rangle, \quad (1.2)$$

where $Y_{lm}(\vartheta, \varphi)$ are the spherical harmonics, we have for ϕ the equation

$$-\phi'' + 2r\phi' + \phi + \frac{l(l+1)}{r^2}\phi = 2E\phi. \quad (1.3)$$

We give in (1.2) the different notations we shall use in these lectures for the single-particle harmonic oscillator states. The index n appearing in them is justified below.

If we try a power-series solution for ϕ ,

$$\phi = r^p \sum_{k=0}^{\infty} a_k r^k, \quad (1.4)$$

we obtain a recursion relation between the a_k :

$$\frac{a_{k+2}}{a_k} = -\frac{(2E-1) - 2(p+k)}{(p+k+2)(p+k+1) - l(l+1)}. \quad (1.5)$$

Let $k = -2, a_{-2} = 0$; then $p(p-1) = l(l+1)$ and hence $p = l+1$, as $p = -l$ is unacceptable because ϕ would diverge at $r = 0$.

We must truncate the series (1.4) at some k_{\max} as this series even when multiplied by $\exp(-\frac{1}{2}r^2)$ does not converge when $r \rightarrow \infty$. Thus,

$$2E - 1 - 2(p + k_{\max}) = 0. \quad (1.6)$$

Since k_{\max} must be even, let $k_{\max} = 2n$. Then,

$$E = 2n + l + \frac{3}{2}, \quad (1.7)$$

and the normalized solution to the radial equation is

$$R_{nl}(r) \equiv \frac{\phi(r)}{r} e^{-\frac{1}{2}r^2} = r^l \sum_{k=0}^n a_{nlk} r^{2k} e^{-\frac{1}{2}r^2}, \quad (1.8)$$

where it may be shown from (1.5) that [1]

$$a_{nlk} = \frac{(-1)^k}{k!} \left[\frac{2(n!)}{\Gamma(n+l+\frac{3}{2})} \right]^{\frac{1}{2}} \frac{\Gamma(n+l+\frac{3}{2})}{(n-k)!\Gamma(k+l+\frac{3}{2})}. \quad (1.9)$$

2 The Matrix Elements of $f(r)Y_{\lambda\mu}(\theta, \varphi)$ with Respect to Harmonic Oscillator States. The Coefficients $B(n'l', nl, p)$

Suppose we wish to find the matrix elements, with respect to states of the harmonic oscillator, of $f(r)Y_{\lambda\mu}(\theta, \varphi)$ where $Y_{\lambda\mu}(\theta, \varphi)$ is a spherical harmonic, i.e., an irreducible Racah tensor of order λ and component μ . From (1.2) and (1.8), the matrix element separates into an angular part and a radial part:

$$\begin{aligned} & \langle n'l'm' | f(r)Y_{\lambda\mu}(\theta, \varphi) | nlm \rangle \\ &= \int \int \int R_{n'l'}(r) Y_{l'm'}^*(\theta, \varphi) f(r) Y_{\lambda\mu}(\theta, \varphi) \\ & \quad \times R_{nl}(r) Y_{lm}(\theta, \varphi) r^2 \sin \theta dr d\theta d\varphi \\ &= \int_0^\infty R_{n'l'}(r) f(r) R_{nl}(r) r^2 dr \langle l'm' | Y_{\lambda\mu}(\theta, \varphi) | lm \rangle. \end{aligned} \quad (2.1)$$

2. THE MATRIX ELEMENTS OF $f(r)Y_{\lambda\mu}(\theta, \varphi)$

By the Wigner-Eckart theorem and the analysis given in Rose [2] one obtains

$$\begin{aligned} & \langle l'm' | Y_{\lambda\mu}(\theta, \varphi) | lm \rangle = \\ & (-1)^{m'} \sqrt{\frac{(2l+1)(2l'+1)(2\lambda+1)}{4\pi}} \begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}, \end{aligned} \quad (2.2)$$

where $\begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix}$ is a $3j$ coefficient. We may evaluate the radial integral by substituting the explicit form (1.8) of R_{nl} into (2.1) and get

$$\begin{aligned} & \int_0^\infty R_{n'l'}(r) f(r) R_{nl}(r) r^2 dr = \\ & \sum_{k=0}^n \sum_{k'=0}^{n'} a_{nlk} a_{n'l'k'} \int_0^\infty r^{2k+2k'+l+l'} f(r) e^{-r^2} r^2 dr. \end{aligned} \quad (2.3)$$

Define

$$p \equiv \frac{1}{2}(2k+2k'+l+l'). \quad (2.4)$$

Note that p ranges from $\frac{1}{2}(l+l')$ to $\frac{1}{2}(l+l') + n + n'$, and the last term in (2.2) implies, from parity considerations, that p is integer (half-integer) if λ is even (odd). Solving for k' we get $k' = p - k - \frac{1}{2}(l+l')$. We may now rewrite (2.3) as

$$\sum_p \sum_k a_{nlk} a_{n'l'p-k-\frac{1}{2}(l+l')} \int_0^\infty r^{2p+2} f(r) e^{-r^2} dr \equiv \sum_p B(n'l', nl, p) I_p, \quad (2.5)$$

where we have defined the B coefficients by

$$B(n'l', nl, p) \equiv \frac{1}{2}\Gamma(p+\frac{3}{2}) \sum_k a_{nlk} a_{n'l'p-k-\frac{1}{2}(l+l')}, \quad (2.6)$$

and I_p is a Talmi integral [3] defined by

$$I_p \equiv \frac{2}{\Gamma(p+\frac{3}{2})} \int_0^\infty r^{2p+2} f(r) e^{-r^2} dr. \quad (2.7)$$

The normalization in (2.7) is chosen so that for $f(r) = 1, I_p = 1$. The coefficients $B(n'l', nl, p)$ have been discussed and tabulated by Brody and Moshinsky [1,4].

The matrix element (2.1) reduces to

$$\begin{aligned} & \langle n'l'm' | f(r) Y_{\lambda\mu}(\theta, \varphi) | nlm \rangle \\ &= \sum_p B(n'l', nl, p) I_p(-1)^{m'} \sqrt{\frac{(2l+1)(2l'+1)(2\lambda+1)}{4\pi}} \\ &\times \begin{pmatrix} l & \lambda & l' \\ m & \mu & -m' \end{pmatrix} \begin{pmatrix} l & \lambda & l' \\ 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (2.8)$$

For convenience we tabulate here the most common Talmi integrals:

$f(r)$	I_p	
r^λ	$\frac{\Gamma(p+\frac{1}{2}\lambda+\frac{3}{2})}{\Gamma(p+\frac{3}{2})}$	(2.9)
$\frac{e^{-\mu r}}{\mu r}$	$\frac{2e^{\mu^2/4}}{\mu\Gamma(p+\frac{3}{2})} \int_{\mu/2}^{\infty} (x - \frac{1}{2}\mu)^{2p+1} e^{-x^2} dx$	(2.10)
$e^{-\alpha^2 r^2}$	$(1 + \alpha^2)^{-p-3/2}$	(2.11)
$\frac{1}{r}$	$\frac{p!}{\Gamma(p+\frac{3}{2})}$	(2.12)

The first one appears when we are dealing with problems involving electric multipoles in which case we have to compute the matrix elements of $r^\lambda Y_{\lambda\mu}(\theta, \varphi)$. The next two appear in nuclear problems when we assume Yukawa or Gaussian interaction between two nucleons. The last one appears for a Coulomb interaction.

3 The One-Electron Atomic Problem. Variational Analysis of the Ground State of the Hydrogen Atom in Terms of Harmonic Oscillator States

All calculations in nuclear physics have two important flaws: (1) one does not use a complete set of basis functions but rather, by introducing models, restricts the basis sufficiently to make calculations feasible; (2) the nuclear Hamiltonian is not known with the precision of other fields in physics.

If the results of calculations differ from experiment, it is not apparent which of the two flaws is at fault. This problem does not exist in atomic or molecular problems, where the Hamiltonian is known exactly. There, if calculations do not agree with experiment, we have made a bad choice

in the selection of the basis functions. We shall therefore apply frequently in these lectures harmonic oscillator states to the description of n -electron atoms or molecules, both for its intrinsic interest and for the insight to the approximation procedure.

We shall neglect the spin-orbit interaction. It is a relativistic effect and, for atoms and molecules of few electrons, is small. The Hamiltonian for a system of n electrons and N nuclei is

$$\begin{aligned} H' = & \sum_{s=1}^n \frac{(p'_s)^2}{2m} + \sum_{s < t=2}^n \frac{e^2}{|\mathbf{x}'_s - \mathbf{x}'_t|} - \sum_{\alpha=1}^N \sum_{s=1}^n \frac{Z_\alpha e^2}{|\mathbf{x}'_s - \mathbf{X}'_\alpha|} \\ & + \sum_{\alpha < \beta=2}^N \frac{Z_\alpha Z_\beta e^2}{|\mathbf{X}'_\alpha - \mathbf{X}'_\beta|}, \end{aligned} \quad (3.1)$$

where \mathbf{x}'_s is the position vector of the s th electron, \mathbf{X}'_α is the position vector of the α th nucleus and Z_α is the charge of nucleus α . The last term in (3.1) gives the repulsion between nuclei and — in the Born-Oppenheimer approximation in which the nuclei are fixed — it is a constant. The constant vectors \mathbf{X}'_α will enter the calculation as variational parameters.

As a trial wave function we shall use a harmonic oscillator wave function of a certain frequency ω , which will be a variational parameter.

Make the change of variables

$$\left. \begin{aligned} x_{is} &= \sqrt{\left(m\omega/\hbar\right)} x'_is \\ X_{i\alpha} &= \sqrt{\left(m\omega/\hbar\right)} X'_i\alpha \\ p_{is} &= (m\omega\hbar)^{-1/2} p'_is \\ H &= \left(me^4/2\hbar^2\right)^{-1} H' \end{aligned} \right\}, \quad (3.2)$$

where $\frac{1}{2}me^4/\hbar^2 \equiv E_B$ is the energy of the first Bohr orbit.

Define a dimensionless parameter

$$\epsilon \equiv \sqrt{\frac{\hbar\omega}{E_B}} = \sqrt{\left[\hbar\omega / \left(\frac{me^4}{2\hbar^2}\right)\right]}. \quad (3.3)$$

Then,

$$H = \frac{1}{2}\epsilon^2 \sum_{s=1}^n (p_s)^2 + \sqrt{2}\epsilon \left[\sum_{s < t=2}^n \frac{1}{|\mathbf{x}_s - \mathbf{x}_t|} \right]$$

$$-\sum_{\alpha=1}^N \sum_{\beta=1}^n \frac{Z_\alpha}{|\mathbf{x}_\beta - \mathbf{X}_\alpha|} + \sum_{\alpha<\beta=2}^N \frac{Z_\alpha Z_\beta}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|}. \quad (3.4)$$

In the case of the hydrogen atom $N = n = 1$ and we choose $X_\alpha = 0$, i.e., we put the nucleus at the origin. Then,

$$H = \frac{1}{2}\epsilon^2 p^2 - \sqrt{2}\epsilon \frac{1}{r}, \quad (3.5)$$

where $r = |\mathbf{x}|$.

The eigenstates ψ of (3.5) have definite l, m and so we could expand them in terms of the corresponding states ψ_{nlm} of (1.2) of the harmonic oscillator, i.e.,

$$\psi = \sum_n a_n |nlm\rangle. \quad (3.6)$$

For a variational analysis of the energy we calculate $\int \psi^* H \psi d\tau$ and minimize this, subject to the constraint $\int \psi^* \psi d\tau = 1$, i.e.,

$$\delta \left[\int \psi^* H \psi d\tau - \lambda \int \psi^* \psi d\tau \right] = 0. \quad (3.7)$$

As from (3.6) ψ is linear in the a 's, this is equivalent to diagonalising $\| \int \psi_{n'l'm}^* H \psi_{nl'm} d\tau \|$ for fixed l, m . The lowest eigenvalue, when minimized with respect to ϵ , will be the energy predicted by the variational procedure for the above trial wave function. As

$$H_{ho} = \frac{1}{2}(p^2 + r^2), \quad (3.8)$$

which implies

$$\frac{1}{2}p^2 = H_{ho} - \frac{1}{2}r^2, \quad (3.9)$$

then

$$\begin{aligned} \langle n'l'm | H | nlm \rangle &= \langle n'l'm | \left(\epsilon^2 H_{ho} - \frac{1}{2}\epsilon^2 r^2 - \sqrt{2}\epsilon \frac{1}{r} \right) | nlm \rangle \\ &= \epsilon^2 (2n + l + \frac{3}{2}) \delta_{n'n} - \frac{1}{2}\epsilon^2 \int_0^\infty R_{n'l}(r) r^4 R_{nl}(r) dr \\ &\quad - \sqrt{2}\epsilon \int_0^\infty R_{n'l}(r) \frac{1}{r} R_{nl}(r) r^2 dr. \end{aligned} \quad (3.10)$$

For the first integral we use the recurrence relations of associate Laguerre polynomials [5]. The second integral may be expanded in terms of Talmi integrals and, using (2.12), we obtain

$$\begin{aligned} \langle n'l'm | H | nlm \rangle &= \frac{1}{2}\epsilon^2 \left\{ [n(n + l + \frac{1}{2})]^{\frac{1}{2}} \delta_{n'n-1} + (2n + l + \frac{3}{2}) \delta_{n'n} \right. \\ &\quad \left. + [(n+1)(n+l+\frac{3}{2})]^{\frac{1}{2}} \delta_{n'n+1} \right\} \\ &\quad - \sqrt{2}\epsilon \sum_{p=l}^{l+n+n'} B(n'l, nl, p) \frac{p!}{\Gamma(p + \frac{3}{2})}. \end{aligned} \quad (3.11)$$

The ground state of the H atom has $l = m = 0$. We need then to calculate the matrix $\| \langle n'00 | H | n00 \rangle \|$. For up to \mathfrak{N} quanta, we would have to diagonalize a $(\frac{1}{2}\mathfrak{N}+1) \times (\frac{1}{2}\mathfrak{N}+1)$ matrix, i.e., $n = 0, 1, \dots, \frac{1}{2}\mathfrak{N}$. Suppose we limit ourselves to zero quanta ($n = n' = 0$); then from the Tables [4] of coefficients B we find

$$\langle H \rangle \equiv \langle 000 | H | 000 \rangle = \frac{3}{4}\epsilon^2 - \sqrt{2}\epsilon B(00, 00, 0) \frac{1}{\Gamma(\frac{3}{2})} = \frac{3}{4}\epsilon^2 - \sqrt{2}\epsilon \frac{2}{\sqrt{\pi}}. \quad (3.12)$$

Minimizing $\langle H \rangle$ with respect to ϵ we get

$$\frac{\partial}{\partial \epsilon} \left[\frac{3}{4}\epsilon^2 - 2\sqrt{\frac{2}{\pi}}\epsilon \right] = \frac{3}{2}\epsilon - 2\sqrt{\frac{2}{\pi}} = 0, \quad (3.13)$$

$$\epsilon = \frac{4}{3}\sqrt{\frac{2}{\pi}} = 1.06. \quad (3.14)$$

From (3.3) $\epsilon = \sqrt{(\hbar\omega/E_B)}$ where $E_B = 13.6$ eV. Thus,

$$\hbar\omega = (1.06)^2 E_B. \quad (3.15)$$

Using the value (3.14) for ϵ the energy is

$$\langle 000 | H | 000 \rangle = -\frac{4}{3} \times \frac{2}{\pi} = -0.849 \quad (3.16)$$

in units of the energy of the first Bohr orbit. Note that this is greater than $-E_B$ as it must be.

If we do the same thing for \mathfrak{N} quanta, keeping ϵ fixed at 1.06, we get [6]

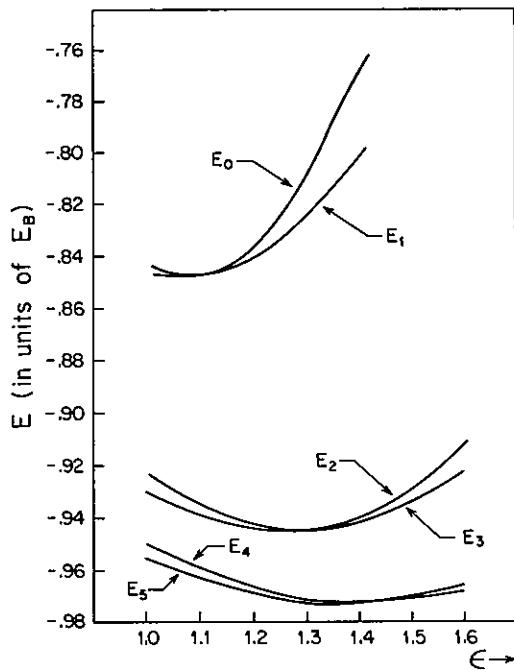


Figure I.1. Energy of the ground state of the H atom as a function of the parameter ϵ for the variational analysis discussed in Section 3. This energy $E_p(\epsilon)$, $p = 0, 1, 2, 3, 4, 5$ is associated with a trial wave function $\psi_p = \sum_{n=0}^p a_n^{(p)} |n00\rangle$, where $|n00\rangle$ is a harmonic-oscillator state of frequency $\hbar\omega = (me^4/2\hbar^2)\epsilon^2$.

Number of quanta	Percentage of binding energy
0	84.9%
2	84.9%
4	93.33%
6	93.73%
8	95.75%
10	96.19%

If — for ten quanta — we vary ϵ , the accuracy increases to 97.35%.

The dependence of the binding energy on ϵ may be seen [7] from Fig. I.1 in which the energies $E_{\mathfrak{N}/2}$ for the \mathfrak{N} -quantum approximation are plotted as a function of ϵ in units of the energy of the first Bohr orbit. As one

3. THE ONE-ELECTRON ATOMIC PROBLEM

increases the number of quanta, the value of ϵ for which the binding energy is minimum increases. In other words, the frequency of the harmonic oscillator for which we get the minimum is increasing.

Note also that the dramatic improvement in the binding energy occurs when one increases the number of quanta by four, rather than by two. This is a general property observed in many calculations [7,8] which we shall prove here rigorously for an arbitrary potential $V(r')$ when we consider its variational analysis for states with $l = m = 0$ and 0+2 quanta, i.e., $n = 0, 1$. The Hamiltonian can then be written as

$$H = \frac{1}{2m} p'^2 + V(r') = \frac{1}{2} \hbar\omega p^2 + V\left(\left[\frac{\hbar}{m\omega}\right]^{\frac{1}{2}} r'\right), \quad (3.17)$$

and its matrix with respect to the above states is

$$\begin{pmatrix} \langle 000|H|000 \rangle & \langle 000|H|100 \rangle \\ \langle 100|H|000 \rangle & \langle 100|H|100 \rangle \end{pmatrix}, \quad (3.18)$$

where

$$\begin{aligned} \langle 000|H|000 \rangle &= \frac{3}{4} \hbar\omega + \frac{4}{\sqrt{\pi}} \int_0^\infty r^2 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right) e^{-r^2} dr \\ &= \frac{3}{4} \hbar\omega + \frac{4}{\sqrt{\pi}} \int_0^\infty \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} r'^2 V(r') \exp\left(-\frac{m\omega}{\hbar} r'^2\right) dr', \end{aligned} \quad (3.19)$$

$$\begin{aligned} \langle 100|H|000 \rangle &= \frac{1}{2} \sqrt{\frac{3}{2}} \hbar\omega + \sqrt{\frac{3}{2}} \frac{4}{\sqrt{\pi}} \int_0^\infty r^2 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right) e^{-r^2} dr \\ &\quad - \sqrt{\frac{3}{2}} \frac{8}{3\sqrt{\pi}} \int_0^\infty r^4 V\left(r\sqrt{\frac{\hbar}{m\omega}}\right) e^{-r^2} dr, \end{aligned} \quad (3.20)$$

and a similar expression for $\langle 100|H|100 \rangle$, all of which can be obtained using the tables of coefficients B of reference [4]. We shall now take the derivative of $\langle 000|H|000 \rangle$, with respect to $\hbar\omega$ and see immediately from (3.19) and (3.20) that

$$\frac{d}{d(\hbar\omega)} \langle 000|H|000 \rangle = \sqrt{\frac{3}{2}} \frac{1}{\hbar\omega} \langle 100|H|000 \rangle. \quad (3.21)$$

It is clear therefore that for the frequency $\hbar\omega$ for which $\langle 000|H|000 \rangle$ is a minimum, i.e., when (3.21) is zero, we have also $\langle 100|H|000 \rangle = 0$; so that there is no improvement for the binding energy when we go from 0 to 0+2 quanta at this frequency. More general relations of this type have been derived by Dubovoy and Flores [8].

4 The One-Electron Molecular Problem. The Ground State of H_2^+ in Terms of Harmonic Oscillator States

From (3.4) we see that the one-electron molecular problem has the Hamiltonian

$$H = \frac{1}{2}\epsilon^2 p^2 - \sqrt{2\epsilon} \left[\sum_{\alpha=1}^N \frac{Z_\alpha}{|\mathbf{x} - \mathbf{X}_\alpha|} - \sum_{\alpha<\beta=2}^N \frac{Z_\alpha Z_\beta}{|\mathbf{X}_\alpha - \mathbf{X}_\beta|} \right]. \quad (4.1)$$

For the discussion of the matrix elements of H with respect to harmonic oscillator states $|nlm\rangle$ we need only analyse the matrix element of $|\mathbf{x} - \mathbf{X}|^{-1}$ with respect to these states when \mathbf{X} is some fixed vector. Denoting by (r, θ, φ) and (R, Θ, Φ) the coordinates of \mathbf{x} and \mathbf{X} respectively, and using the expansion

$$\frac{1}{|\mathbf{x} - \mathbf{X}|} = \sum_{k=0}^{\infty} \left[\frac{r^k / R^{k+1}}{R^k / r^{k+1}} \right] \frac{4\pi}{2k+1} \sum_{q=-k}^k Y_{kq}^*(\Theta, \Phi) Y_{kq}(\theta, \varphi), \quad (4.2)$$

where upper (lower) terms in the square brackets are employed according to whether $r \leq R$ ($r > R$), the matrix element of $|\mathbf{x} - \mathbf{X}|^{-1}$ reduces to a linear combination of matrix elements of the form

$$\begin{aligned} \langle n'l'm' | & \left[\frac{r^k / R^{k+1}}{R^k / r^{k+1}} \right] Y_{kq}(\theta, \varphi) | nlm \rangle \\ &= \langle n'l' | \left[\frac{r^k / R^{k+1}}{R^k / r^{k+1}} \right] Y_k(\theta, \varphi) | nl \rangle (-1)^{l-k+m'} \\ &\quad \times \sqrt{2l'+1} \begin{pmatrix} l & k & l' \\ m & q & -m' \end{pmatrix} \\ &= \sum_p \left\{ B(n'l', nl, p) I_p^k(R) (-1)^{m'} \begin{pmatrix} l & k & l' \\ m & q & -m' \end{pmatrix} \right. \\ &\quad \left. \times \begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix} \sqrt{\frac{(2l+1)(2l'+1)(2k+1)}{4\pi}} \right\}, \quad (4.3) \end{aligned}$$

where

$$\begin{aligned} I_p^k(R) &\equiv \frac{2}{\Gamma(p + \frac{3}{2})} \left[\int_0^R \frac{r^{2p+k+2}}{R^{k+1}} e^{-r^2} dr + \int_R^\infty R^k r^{2p-k+1} e^{-r^2} dr \right] \\ &= \frac{1}{\Gamma(p + \frac{3}{2})} \left\{ \left[\sum_{q=0}^{p-\frac{1}{2}k} R^{2q+k} \frac{(p - \frac{1}{2}k)!}{q!} \right. \right. \\ &\quad \left. \left. - \sum_{q=0}^{p+\frac{1}{2}k} \frac{R^{2q-k} (2p+k+1)!!}{2^{p-q+\frac{1}{2}k} (2q+1)!!} \right] e^{-R^2} \right. \\ &\quad \left. + \frac{\sqrt{\pi}(2p+k+1)!!}{R^{k+1} 2^{p+1+\frac{1}{2}k}} \text{erf}(R) \right\}. \quad (4.4) \end{aligned}$$

In (4.4) $\text{erf}(R)$ stands for the error function

$$\text{erf}(R) \equiv \frac{2}{\sqrt{\pi}} \int_0^R e^{-t^2} dt. \quad (4.5)$$

From the selection rule implied by the coefficient $\begin{pmatrix} l & k & l' \\ 0 & 0 & 0 \end{pmatrix}$ in Eq. (4.3), i.e., $l + l' + k$ even, and from the restriction on the values of p implied in (2.4), we conclude that $p \pm \frac{1}{2}k$ in (4.4) is always an integer.

Particularizing the Hamiltonian (4.1) to the H_2^+ molecule, we could take the two protons with coordinates $\mathbf{X}_1 = \mathbf{X}$, $\mathbf{X}_2 = -\mathbf{X}$, \mathbf{X} being a vector along the z-axis of magnitude, R , $2R$ being the intermolecular distance. If we then take the expectation value of H with respect to a zero-quantum harmonic oscillator state, we obtain

$$\langle H \rangle = \langle 000 | H | 000 \rangle = \frac{3}{4}\epsilon^2 + \epsilon f(R), \quad (4.6)$$

with

$$f(R) = \frac{1}{R\sqrt{2}} [1 - 4 \text{erf}(R)]. \quad (4.7)$$

We shall choose for ϵ the value that minimizes $\langle H \rangle$ when we take for R the value R_0 which gives the lowest value for $\langle H \rangle$, i.e., ϵ and R_0 are determined by the equations

$$\frac{\partial}{\partial \epsilon} \langle H \rangle = \frac{3}{2}\epsilon + f(R) = 0, \quad \frac{\partial}{\partial R} \langle H \rangle = \epsilon \frac{df}{dR} = 0. \quad (4.8)$$

The value R_0 is obtained by drawing $f(R)$ and seeking its minimum, while ϵ is given by $\epsilon = -\frac{2}{3}f(R_0)$. Thus we finally get for $\langle H \rangle$ the expression

$$\langle H \rangle_{\min} \equiv E(R) = \frac{1}{3}f(R_0)[f(R_0) - 2f(R)]. \quad (4.9)$$

In Fig. I.2 we give $E(R)$ for H_2^+ as compared with the exact calculation. The total electronic energy we get at the minimum of the curve is 84% of

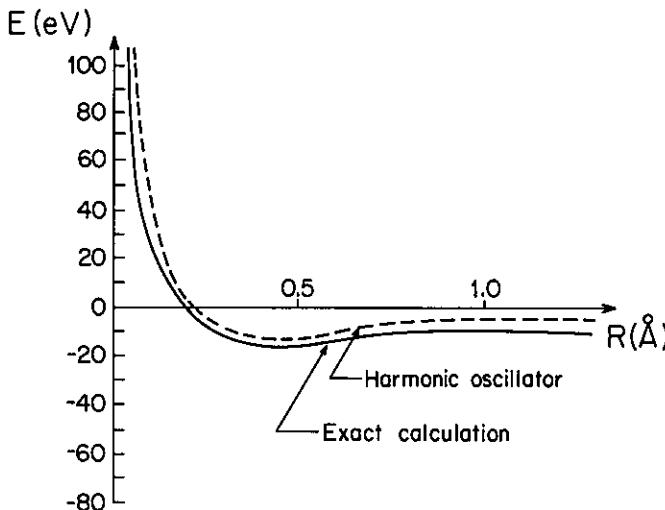


Figure I.2. Expectation value $E(R)$ of the Hamiltonian of the H_2^+ molecule as a function of R , half the internuclear distance. The single-electron wave function is represented by a zero-quantum state of the harmonic oscillator, whose frequency is chosen so as to minimize the energy $E(R)$.

the experimental value and the theoretical internuclear distance is 1.022 Å, while the experimental one is 1.06 Å.

For H_2^+ Bender [9] has carried out calculations with harmonic oscillator functions of up to four quanta. In his analysis he deals with electronic energies, *i.e.*, he does not include the term of nuclear repulsion. Taking the results of Bender for the experimental $R = 0.53$ Å with the value for the frequency of the oscillator that minimizes the energy for the given R , and adding $e^2/2R$, one gets the following:

- The calculated energy for the state $|000\rangle$ is 84% of the experimental one, coinciding with the above analysis, as of course it should.
- For a linear combination of the states $|000\rangle$ and $|100\rangle$ the calculated energy is 88.66% of the exact value.
- For a linear combination of $|000\rangle$ and $|020\rangle$ the calculated energy is 88.88% of the exact value.
- For the following combination

$$a_1|000\rangle + a_2|100\rangle + a_3|020\rangle + a_4|200\rangle + a_5|120\rangle + a_6|040\rangle, \quad (4.10)$$

which corresponds to an approximation of up to four quanta, one gets from Bender's analysis 93.46% of the exact energy and the following values for the coefficients:

$$\left. \begin{array}{l} a_1 = 0.96396 \quad a_3 = 0.15880 \quad a_5 = 0.06226 \\ a_2 = -0.18707 \quad a_4 = 0.07847 \quad a_6 = 0.02334 \end{array} \right\}. \quad (4.11)$$

We see that the convergence with increasing number of quanta for H_2^+ is as good as for H.

5 Scattering of Electrons by Hydrogen Atoms and the Form Factor of the Electron-Charge Distribution in the Ground State

We have used harmonic oscillator states for a variational analysis of the ground state of the hydrogen atom. In the following sections we shall employ them in the analysis of the form factor of the hydrogen atom to establish the basis for a similar analysis later on of the form factor of the 3H nucleus considered as a three nucleon system and of the α particle as a four-nucleon system.

We first indicate how one could derive experimentally the form factor from the differential elastic scattering cross section of electrons by hydrogen atoms. For high (but still non-relativistic) energies the differential scattering cross section could be given by the Born approximation [10]*

$$d\sigma = \frac{m^2}{4\pi^2\hbar^4} \left| \int U(r') \exp(i\mathbf{q} \cdot \mathbf{r}') dr' \right|^2 d\Omega, \quad (5.1)$$

where m is the electron mass, $d\Omega$ the differential solid angle and $\hbar\mathbf{q}$ the momentum transfer

$$\hbar\mathbf{q} = \mathbf{p}' - \bar{\mathbf{p}}',$$

or, as $\mathbf{p}' = \bar{\mathbf{p}}'$,

$$\hbar\mathbf{q} = 2\mathbf{p}' \sin \frac{1}{2}\theta, \quad (5.2)$$

*We use always r', p' , etc. to indicate coordinates and momenta in ordinary units and reserve r, p for the corresponding dimensionless quantities.

where θ is the scattering angle. In (5.1) $U(r')$ can be taken as the sum of the potential due to the proton plus the one due to the electron charge distribution, *i.e.*,

$$U(r') = -\frac{e^2}{r'} + e^2 \int \frac{\rho(\mathbf{r}'')}{|\mathbf{r}' - \mathbf{r}''|} d\mathbf{r}'', \quad (5.3)$$

where $\rho(\mathbf{r}')$ is given in terms of the ground state wave function ψ by

$$\rho(\mathbf{r}') = \psi^*(\mathbf{r}')\psi(\mathbf{r}'). \quad (5.4)$$

Making use of the convolution theorem [11] that states

$$\int dx e^{ikx} \int dy f(x-y)g(y) = \int dx e^{ikx} f(x) \int dy e^{iky} g(y), \quad (5.5)$$

we obtain

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{m^2}{4\pi^2 \hbar^4} \left| \int \left[\frac{e^2}{r'} - \int \frac{e^2 \rho(\mathbf{r}'')}{|\mathbf{r}' - \mathbf{r}''|} d\mathbf{r}'' \right] \exp(i\mathbf{q} \cdot \mathbf{r}') d\mathbf{r}' \right|^2 \\ &= \left(\frac{d\sigma}{d\Omega} \right)_R \left| 1 - \int \rho(\mathbf{r}') \exp(i\mathbf{q} \cdot \mathbf{r}') d\mathbf{r}' \right|^2, \end{aligned} \quad (5.6)$$

where

$$\left(\frac{d\sigma}{d\Omega} \right)_R = \frac{m^2}{4\pi^2 \hbar^4} \left| \int \frac{e^2}{r'} \exp(i\mathbf{q} \cdot \mathbf{r}') d\mathbf{r}' \right|^2 \quad (5.7)$$

is the Rutherford scattering cross section.

From (5.6) we see that

$$1 - \left[\left(\frac{d\sigma}{d\Omega} \right) / \left(\frac{d\sigma}{d\Omega} \right)_R \right]^{\frac{1}{2}} = \int \rho(\mathbf{r}') \exp(i\mathbf{q} \cdot \mathbf{r}') d\mathbf{r}' \equiv F(\mathbf{q}), \quad (5.8)$$

where $F(\mathbf{q})$ is the form factor for the electron charge distribution in the ground state of the hydrogen atom. From the experimental information on the ratio of the differential elastic cross section to the Rutherford differential cross section, we can therefore obtain information on $F(\mathbf{q})$ and, from (5.8) and (5.4), on the ground-state wave function $\psi(\mathbf{r}')$.

Of course, in the case of the hydrogen atom we know the wave function for the ground state:

$$\psi(r') = \frac{1}{\sqrt{(\pi a^3)}} \exp\left(-\frac{r'}{a}\right), \quad (5.9)$$

where $a = \hbar^2/me^2$ is the Bohr radius; so the exact form factor $F_e(\mathbf{q})$ is

$$\begin{aligned} F_e(\mathbf{q}) &= \frac{1}{\pi a^3} \int \exp\left(-\frac{2r'}{a}\right) \exp(i\mathbf{q} \cdot \mathbf{r}') d\mathbf{r}' \\ &= \frac{4}{a^3} \int_0^\infty \exp\left(-\frac{2r'}{a}\right) \frac{\sin qr'}{qr'} r'^2 dr', \end{aligned} \quad (5.10)$$

which is a function of q^2 only:

$$F_e(q^2) = \left[1 + \left(\frac{aq}{2} \right)^2 \right]^{-2}. \quad (5.11)$$

In the next section we shall derive an expression for the form factor when we use harmonic oscillator functions to describe the ground state of the hydrogen atom. We shall then compare the results for different number of quanta in the approximation with the exact result.

6 Theoretical Form Factor of the Hydrogen Atom Using Harmonic Oscillator States

Suppose we do not know the exact wave function for the ground state of the hydrogen atom but that we could approximate it in terms of harmonic oscillator functions for up to N quanta, *i.e.*,

$$\psi = \sum_n a_n |n00\rangle = \frac{1}{\sqrt{(4\pi)}} \sum_n a_n R_{n0}(r), \quad n = 0, 1, \dots, \frac{1}{2}N. \quad (6.1)$$

In this equation r is the dimensionless one of section 1. The coefficients a_n can be determined from the variational analysis discussed in (3.7), which leads to the following set of linear equations for a_n :

$$\sum_n \langle n'00 \left| \frac{1}{2} \epsilon^2 p^2 - \frac{\sqrt{2}\epsilon}{r} \right| n00 \rangle a_n = E(\epsilon) a_{n'}. \quad (6.2)$$

Here $E(\epsilon)$, the lowest eigenvalue for the matrix of the Hamiltonian in (6.2), is the function of ϵ plotted in Fig. I.1. If we take for ϵ the value that gives the minimum of $E(\epsilon)$ for $N = 0, 2, 4, 6, 8$ or 10 quanta, we can obtain the corresponding a_n for these cases.

The charge density associated with the ψ of (6.1) is given by

$$\rho(r) = \frac{1}{4\pi} \sum_{nn'} a_{n'}^* a_n R_{n'0}(r) R_{n0}(r), \quad (6.3)$$

and so the corresponding form factor is, from (5.8),

$$\begin{aligned} F(q^2) &= \int \exp(i\kappa \cdot \mathbf{r}) \rho(\mathbf{r}) d\mathbf{r} \\ &= 4\pi \int_0^\infty \rho(r) \frac{\sin \kappa r}{\kappa r} r^2 dr = \sum_{n'n} a_{n'}^* a_n M_{n'n}(\kappa^2). \end{aligned} \quad (6.4)$$

In (6.4) κ^2 is related to q^2 by

$$\kappa^2 = \frac{\hbar}{m\omega} q^2 = 2 \left(\frac{\hbar^2}{me^2} \right)^2 \frac{1}{\epsilon^2} q^2, \quad (6.5)$$

as the \mathbf{r} in the integral is dimensionless. Furthermore,

$$M_{n'n}(\kappa^2) \equiv \int_0^\infty R_{n'0}(r) \frac{\sin \kappa r}{\kappa r} R_{n0}(r) r^2 dr = \sum_{p=0}^{n'+n} B(n'0, n0, p) I_p(\kappa^2), \quad (6.6)$$

with

$$\begin{aligned} I_p(\kappa^2) &= \frac{2}{\Gamma(p + \frac{3}{2})} \int_0^\infty r^{2p+2} \frac{\sin \kappa r}{\kappa r} e^{-r^2} dr \\ &= \frac{1}{2} e^{-\kappa^2/4} \sum_{s=0}^p \binom{2p+1}{2s} \frac{\Gamma(s + \frac{1}{2})}{\Gamma(p + \frac{3}{2})} \left(-\frac{\kappa^2}{4} \right)^{p-s}, \end{aligned} \quad (6.7)$$

as can be easily seen by integration by parts.

Using for a_n the values obtained by this variational procedure for $N = 0, 4$ and 8 and taking the appropriate value of ϵ in (6.5) for these three cases, Yeh [12] computed the corresponding form factors; they are plotted in Fig. I.3, where he also plotted the exact form factor $F_e(q^2)$. Note that the curves are plotted in a semilogarithmic scale, so that in the zero-quantum approximation we get just a straight line. From the figure we see clearly that we can approach the exact form factor as closely as we want if we increase the number of quanta N in the analysis.

6. THEORETICAL FORM FACTOR

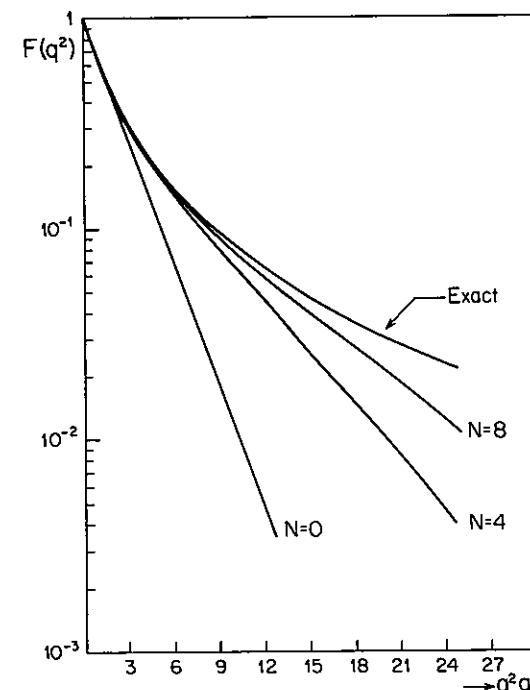


Figure I.3. Form factor for the electronic charge of the ground state of the H atom as a function of the square of the momentum transfer q^2 . The upper line is the exact form factor (5.11). The other lines are the form factors (6.4) for the linear combination of harmonic-oscillator states obtained by the variational analysis of §3. The notation $N = 0, 4, 8$ stands for the maximum number of quanta in the expansion.

In Fig. I.3 we included only the form factor for expansions of ψ that differ by jumps of four quanta, for the reasons stressed at the end of section 3.

In the next section we discuss an alternative procedure for getting the a_n directly from the experiment, or in the case of the hydrogen atom the exact, form factor, thus bypassing the variational analysis of this section which requires the knowledge of the Hamiltonian in (6.2).

7 Direct Determination of the Ground State Through a Least-Squares Approach to the Form Factor. The Pseudo Hartree-Fock (PHF) Approximation

Suppose that we do not know the potential in the hydrogen atom but that we have at our disposal the experimental data for the form factor taken from the elastic scattering of electrons by hydrogen atoms. These experimental results will be assumed here to be the same as Eq. (5.11), i.e., $F_e(q^2) = [1 + (qa/2)^2]^{-2}$, since this is the exact form factor.

Consider now the derivative of $F_e(q^2)$ with respect to q^2 computed at the point $q^2 = 0$. This gives us the slope of $F_e(q^2)$ at $q^2 = 0$. We shall show that this slope is proportional to the mean square radius and later use this result to fix the frequency of the harmonic oscillator states we require. To obtain the derivative dF/dq^2 we see from Eq. (6.4) that essentially we have to calculate

$$\frac{d}{dq^2} \frac{\sin qr'}{qr'} = \frac{1}{2q} \frac{d}{dq} \frac{\sin qr'}{qr'} = \frac{1}{2q^2} \left(\cos qr' - \frac{\sin qr'}{qr'} \right). \quad (7.1)$$

Expanding $\cos qr'$ and $\sin qr'/qr'$ in power series we get finally

$$\left[\frac{d}{dq^2} \frac{\sin qr'}{qr'} \right]_{q^2=0} = -\frac{1}{6} r'^2, \quad (7.2)$$

so that

$$\left(\frac{dF}{dq^2} \right)_{q^2=0} = -\frac{4\pi}{6} \int_0^\infty \rho(r') r'^4 dr'. \quad (7.3)$$

Now the $\rho(r')$ associated with $F_e(q^2)$ is $(\pi a^3)^{-1} \exp(-2r'/a)$ so that

$$\left(\frac{dF_e}{dq^2} \right)_{q^2=0} = -\frac{1}{2} a^2. \quad (7.4)$$

Note that this result could be obtained directly from (5.11); however, Eq. (7.3) holds for the $\rho(r')$ associated with any wave function describing the ground state of the hydrogen atom. We shall use it with the harmonic oscillator expression (6.1) and then compare with (7.4). In this way we shall fix ϵ .

With a harmonic oscillator of zero quanta we get

$$\rho(r) = \pi^{-\frac{3}{2}} e^{-r^2}, \quad (7.5)$$

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where now r is the dimensionless variable of section 1. Putting this $\rho(r)$ into Eq. (7.3) we obtain

$$\left(\frac{dF}{dq^2} \right)_0 = \frac{\hbar}{m\omega} \left(\frac{dF}{d\kappa^2} \right)_0 = \frac{\hbar}{m\omega} \left[-\frac{4\pi}{6} \int_0^\infty r^4 \pi^{-\frac{3}{2}} e^{-r^2} dr \right] = -\frac{1}{4} \frac{\hbar}{m\omega}, \quad (7.6)$$

where we have used the relation between κ^2 and q^2 of (6.5) which is needed for the dimensionless r . Equating this result with the "experimental" value of Eq. (7.4), we have

$$\frac{1}{4} \frac{\hbar}{m\omega} = \frac{1}{2} a^2 = \frac{1}{2} \frac{\hbar^4}{m^2 e^4}, \quad (7.7)$$

or

$$\frac{\hbar\omega}{(me^4/2\hbar^2)} = \epsilon = 1. \quad (7.8)$$

Thus from the form factor we have determined the value 1 for our parameter ϵ . This is in good agreement with the variational analysis in the zero-quantum approximation, where we get $\epsilon = 1.06$ [see Eq. (3.13)].

To define completely the wave function of Eq. (6.1) there remains the problem of determining the coefficients a_n . We shall do this by a least-squares fitting of the $F(q^2)$ of (6.4) to the $F_e(q^2)$ subject to the constraint that ψ is normalized; i.e., we shall minimize the expression

$$\int_0^\infty [F(q^2) - F_e(q^2)]^2 dq^2 - \lambda \sum_n a_n^* a_n, \quad n = 0, 1, \dots, \frac{1}{2}\mathfrak{N}, \quad (7.9)$$

where λ is a Lagrange multiplier. From (6.4) this expression becomes

$$\begin{aligned} & \sum_{n'n}^{n'm} a_n^* a_m^* a_n a_m \int_0^\infty M_{n'n}(q^2) M_{m'm}(q^2) dq^2 \\ & - 2 \sum_{n'n}^{n'm} a_n^* a_n \int_0^\infty M_{n'n}(q^2) F_e(q^2) dq^2 \\ & + \int_0^\infty [F_e(q^2)]^2 dq^2 - \lambda \sum_{n'n} a_n^* a_n \delta_{n'n}. \end{aligned} \quad (7.10)$$

All sums go from 0 to $\frac{1}{2}\mathfrak{N}$, and $M_{n'n}(q^2)$ are given by (6.6), so that taking its derivative with respect to a_k^* we obtain the following system of algebraic equations:

$$2 \sum_n \left[\sum_{m'm} a_{m'}^* a_m \int_0^\infty M_{kn}(q^2) M_{m'm}(q^2) dq^2 \right] a_n - 2 \sum_n \left[\int_0^\infty M_{kn}(q^2) F_e(q^2) dq^2 \right] a_n = \lambda a_k. \quad (7.11)$$

We solve (7.11) by successive approximations. Starting with a first guess $a_n^{(0)}$, we use (6.4) to define, from the $(p-1)$ th approximation $a_n^{(p-1)}$, the quantity

$$F^{(p-1)}(q^2) \equiv \sum_{m'm} a_{m'}^{*(p-1)} a_m^{(p-1)} M_{m'm}(q^2). \quad (7.12)$$

Substituting in (7.11), we obtain a set of equations which is linear:

$$2 \sum_n \left[\int_0^\infty dq^2 [F^{(p-1)}(q^2) - F_e(q^2)] M_{kn}(q^2) \right] a_n^{(p)} = \lambda a_k^{(p)}. \quad (7.13)$$

We continue this process until (7.13) has a self-consistent solution, i.e., until $a_n^{(p)} = a_n^{(p-1)}$ to the approximation desired.

Equations (7.11) and the method we propose for solving them are very similar to those used in the Hartree-Fock approximation [13], which is why we shall refer to this procedure of getting the coefficients a_n , as the Pseudo Hartree-Fock (PHF) approximation.

Equations (7.13) were solved by A.M. Cetto [14] for $N = 2$ and $\epsilon = 1$; she obtained the following results:

$$\begin{aligned} a_0^{(0)} &= 1 & a_0^{(1)} &= 0.680 & a_0^{(2)} &= 0.650 \\ a_1^{(0)} &= 0 & a_1^{(1)} &= 0.733 & a_1^{(2)} &= 0.760 \end{aligned} \quad (7.14)$$

Thus self-consistency was practically achieved after two steps [14].

8 The One-Body Harmonic Oscillator States Expressed in Terms of Creation Operators

If we have a one-dimensional harmonic oscillator we know that the states are characterized by an integer quantum number n and can be expressed in terms of a creation operator applied to the ground state in the following way:

$$|n\rangle = \frac{1}{\sqrt{n!}} \eta^n |0\rangle, \quad |0\rangle = \pi^{-\frac{3}{4}} e^{-\frac{1}{2}x^2}, \quad (8.1)$$

where

$$\eta = \frac{1}{\sqrt{2}}(x - ip) = \frac{1}{\sqrt{2}} \left(x - \frac{d}{dx} \right). \quad (8.2)$$

It is easy to prove that $|n\rangle$ is an eigenstate of H :

$$H|n\rangle = \frac{1}{2}(p^2 + x^2)|n\rangle = (n + \frac{1}{2})|n\rangle. \quad (8.3)$$

In order to see this, define the annihilation operator

$$\xi = \eta^\dagger = \frac{1}{\sqrt{2}}(x + ip) = \frac{1}{\sqrt{2}} \left(x + \frac{d}{dx} \right), \quad (8.4)$$

so that from (8.1) we obtain

$$\xi|0\rangle = \frac{1}{\sqrt{2}} \left(x + \frac{d}{dx} \right) \pi^{-\frac{3}{4}} e^{-\frac{1}{2}x^2} = \frac{\pi^{-\frac{1}{4}}}{\sqrt{2}} x [e^{-\frac{1}{2}x^2} - e^{-\frac{1}{2}x^2}] = 0. \quad (8.5)$$

On the other hand we have the commutator $[\xi, \eta] = 1$, so that

$$\begin{aligned} H|n\rangle &= \frac{1}{2}(p^2 + x^2)|n\rangle = (\eta\xi + \frac{1}{2})|n\rangle = \eta\xi \frac{1}{\sqrt{n!}} \eta^n |0\rangle + \frac{1}{2}|n\rangle \\ &= \frac{1}{\sqrt{n!}} \eta[\xi, \eta^n]|0\rangle + \frac{1}{2}|n\rangle = \frac{n}{\sqrt{n!}} \eta^n |0\rangle + \frac{1}{2}|n\rangle = (n + \frac{1}{2})|n\rangle, \end{aligned} \quad (8.6)$$

where we have used the result $[\xi, \eta^n] = n\eta^{n-1}$.

The generalization for three dimensions is immediate. In this case the functions are given by

$$|n_1 n_2 n_3\rangle = [n_1! n_2! n_3!]^{-\frac{1}{2}} \eta_1^{n_1} \eta_2^{n_2} \eta_3^{n_3} |0\rangle, \quad (8.7)$$

with

$$\eta_j = \frac{1}{\sqrt{2}}(x_j - ip_j), \quad \xi_j = \eta_j^\dagger, \quad j = 1, 2, 3. \quad (8.8)$$

Now the normalized ground state is described by

$$|0\rangle = \pi^{-\frac{3}{4}} \exp[-\frac{1}{2}(x_1^2 + x_2^2 + x_3^2)]. \quad (8.9)$$

In these coordinates (Cartesian) the quantum numbers are n_1, n_2 and n_3 , associated with the integrals of motion H_1, H_2 and H_3 . The states (8.7) in general are not eigenstates of L^2 or L_3 . If we want to characterize the states in terms of the eigenvalues of H, L^2 and L_3 , namely N, l, m we have

to obtain appropriate homogeneous polynomials of degree N in the η_i 's. To derive them we first discuss the following auxiliary problem: What is the polynomial $P = P(x_1, x_2, x_3)$ that satisfies the equations

$$\left. \begin{aligned} \mathbf{r} \cdot \nabla P &= NP \\ \mathbf{L}^2 P &= l(l+1)P \\ L_3 P &= mP \end{aligned} \right\}, \quad (8.10)$$

with N, l, m integers, $-l \leq m \leq l, N \geq l$ and $N - l$ even? Clearly it is the homogeneous polynomials of degree $N, r^N Y_{lm}(\theta, \varphi)$, where Y_{lm} is the usual spherical harmonic. Introducing the concept of solid spherical harmonic

$$\mathcal{Y}_{lm}(\mathbf{x}) \equiv r^l Y_{lm}(\theta, \varphi), \quad (8.11)$$

the solution could also be written as

$$(\mathbf{x} \cdot \mathbf{x})^n \mathcal{Y}_{lm}(\mathbf{x}), \quad \text{with } N = 2n + l. \quad (8.12)$$

Let us now return to the creation and annihilation operators η_i, ξ_j . From (8.8) it is easy to see that

$$[\xi_i, \eta_j] = \delta_{ij}, \quad [\xi_i, \xi_j] = [\eta_i, \eta_j] = 0, \quad (8.13)$$

and

$$\boldsymbol{\eta} \times \boldsymbol{\xi} = \frac{1}{2}i(\mathbf{x} \times \mathbf{p} - \mathbf{p} \times \mathbf{x}) = i\mathbf{x} \times \mathbf{p}, \quad (8.14)$$

so that

$$\mathbf{L} = -i\boldsymbol{\eta} \times \boldsymbol{\xi}. \quad (8.15)$$

From (8.13) we conclude that ξ_j , when acting on a polynomial in the creation operators η_j can be interpreted as the operator $\partial/\partial\eta_j$, for the same reasons that $p = -i\partial/\partial x_j$. It is clear therefore from (8.10) and (8.12) that the state

$$|nlm\rangle \equiv A_{nl}(\boldsymbol{\eta} \cdot \boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle, \quad (8.16)$$

in which A_{nl} is a normalization constant, satisfies the equations

$$\left. \begin{aligned} (H - \frac{3}{2})|nlm\rangle &= \boldsymbol{\eta} \cdot \boldsymbol{\xi}|nlm\rangle = N|nlm\rangle \\ L^2|nlm\rangle &= l(l+1)|nlm\rangle \\ L_3|nlm\rangle &= m|nlm\rangle \end{aligned} \right\}. \quad (8.17)$$

Thus $|nlm\rangle$, defined by (8.16), is simultaneously an eigenfunction of H, L^2, L_3 , and is given in terms of a definite homogeneous polynomial of degree $N = 2n + l$ in the η_j applied to the ground state:

$$|0\rangle \equiv \pi^{-\frac{3}{4}} e^{-\frac{1}{2}r^2}. \quad (8.18)$$

The normalization coefficient A_{nl} , derived in the next section, is

$$A_{nl} = (-1)^n \left[\frac{4\pi}{(2n+2l+1)!!(2n)!!} \right]^{\frac{1}{2}}. \quad (8.19)$$

9 Normalization Coefficients of the Harmonic Oscillator States

The normalization constant A_{nlm} may be calculated by computing the scalar product of $|nlm\rangle$ with itself:

$$1 = \langle nlm|nlm\rangle = |A_{nlm}|^2 \langle 0|\mathcal{Y}_{lm}^\dagger(\boldsymbol{\eta})(\boldsymbol{\xi} \cdot \boldsymbol{\xi})^n (\boldsymbol{\eta} \cdot \boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle. \quad (9.1)$$

The first step is to develop a recursion relation in n which enables us to relate this matrix element to that for $n = 0$, which may then be easily evaluated. From the correspondence $\xi_j \rightarrow \partial/\partial\eta_j$ we see that $\boldsymbol{\xi} \cdot \boldsymbol{\xi}$ will operate on $(\boldsymbol{\eta} \cdot \boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})$ in the same way as the Laplacian

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{r^2} \quad (9.2)$$

does on $(\mathbf{x} \cdot \mathbf{x})^n \mathcal{Y}_{lm}(\mathbf{x})$; this is found easily:

$$\begin{aligned} \nabla^2(\mathbf{x} \cdot \mathbf{x})^n \mathcal{Y}_{lm}(\mathbf{x}) &= \nabla^2 r^{2n+l} Y_{lm}(\theta, \varphi) \\ &= [(2n+l)(2n+l+1) - l(l+1)] r^{2n-2} \mathcal{Y}_{lm}(\mathbf{x}) \\ &= 2n(2n+2l+1) r^{2n-2} \mathcal{Y}_{lm}(\mathbf{x}). \end{aligned} \quad (9.3)$$

Using this analogy, the scalar product (9.1) becomes

$$\begin{aligned} \langle 0|\mathcal{Y}_{lm}^\dagger(\boldsymbol{\eta})(\boldsymbol{\xi} \cdot \boldsymbol{\xi})^n (\boldsymbol{\eta} \cdot \boldsymbol{\eta})^n \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle \\ = 2n(2n+2l+1) \langle 0|\mathcal{Y}_{lm}^\dagger(\boldsymbol{\eta})(\boldsymbol{\xi} \cdot \boldsymbol{\xi})^{n-1} (\boldsymbol{\eta} \cdot \boldsymbol{\eta})^{n-1} \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle \\ = \frac{(2n)!!(2n+2l+1)!!}{(2l+1)!!} \langle 0|\mathcal{Y}_{lm}^\dagger(\boldsymbol{\eta}) \mathcal{Y}_{lm}(\boldsymbol{\eta})|0\rangle. \end{aligned} \quad (9.4)$$

The analysis is now simplified by noting that the scalar product in (9.4) is independent of m . This can be seen as follows: recall that

$$L_+|0lm\rangle = [(l-m)(l+m+1)]^{\frac{1}{2}}|0lm+1\rangle \quad (9.5)$$

or

$$[(l-m)(l+m+1)]^{-\frac{1}{2}}L_+|0lm\rangle = |0lm+1\rangle. \quad (9.6)$$

Thus, we have

$$\langle 0|\mathcal{Y}_{lm+1}^\dagger \mathcal{Y}_{lm+1}|0\rangle = [(l-m)(l+m+1)]^{-1} \langle 0|\mathcal{Y}_{lm}^\dagger L_- L_+ \mathcal{Y}_{lm}|0\rangle. \quad (9.7)$$

Using $L^2 = L_- L_+ + L_0(L_0 + 1)$, we obtain

$$\langle 0|\mathcal{Y}_{lm+1}^\dagger \mathcal{Y}_{lm+1}|0\rangle = \frac{l(l+1) - m(m+1)}{(l-m)(l+m+1)} \langle 0|\mathcal{Y}_{lm}^\dagger \mathcal{Y}_{lm}|0\rangle = \langle 0|\mathcal{Y}_{lm}^\dagger \mathcal{Y}_{lm}|0\rangle, \quad (9.8)$$

which is the desired result. We may now drop the m index on A_{nlm} , as was already done in (8.16).

Thus we may choose, without loss of generality $m = l$; $\mathcal{Y}_{lm}(x)$ then reduces to [15]

$$\begin{aligned} \mathcal{Y}_l(r) &= (-)^l \sqrt{\left(\frac{(2l+1)!}{2}\right)} \frac{r^l}{l! 2^l} \sin^l \theta \frac{1}{\sqrt{(2\pi)}} e^{il\varphi} \\ &= \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} (x_+)^l, \end{aligned} \quad (9.9)$$

where

$$x_\pm \equiv \mp \frac{1}{\sqrt{2}}(x_1 \pm ix_2). \quad (9.10)$$

In analogy we have

$$\mathcal{Y}_l(\eta) = \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} (\eta_+)^l, \quad (9.11)$$

where

$$\eta_\pm \equiv \mp \frac{1}{\sqrt{2}}(\eta_1 \pm i\eta_2). \quad (9.12)$$

Then,

$$\langle 0|\mathcal{Y}_l^\dagger(\eta) \mathcal{Y}_l(\eta)|0\rangle = \frac{(2l+1)!}{4\pi} \frac{1}{2^l (l!)^2} \langle 0|(\eta_+^\dagger)^l (\eta_+)^l|0\rangle = \frac{(2l+1)!!}{4\pi}. \quad (9.13)$$

Using (9.4) and (9.13), (9.1) becomes

9. NORMALIZATION COEFFICIENTS

$$\langle nlm|nlm\rangle = |A_{nl}|^2 \frac{(2n)!!(2n+2l+1)!!}{(2l+1)!!} \frac{(2l+1)!!}{4\pi}, \quad (9.14)$$

or

$$A_{nl} = e^{i\delta_{nl}} \left[\frac{4\pi}{(2n)!!(2n+2l+1)!!} \right]^{\frac{1}{2}}. \quad (9.15)$$

We shall choose the phase factor $e^{i\delta_{nl}}$ to conform with the standard definition of the associated Laguerre polynomial [16] in which the coefficient a_{nl0} of (1.8) is positive.

From (1.8) and (9.9) we see that

$$|nll\rangle = \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} x_+^l \sum_{k=0}^n a_{nlk} r^{2k} e^{-\frac{1}{2}r^2}, \quad (9.16)$$

with a_{nlk} given by (1.9), while in terms of creation operators $|nll\rangle$ is given by

$$|nll\rangle = A_{nl} \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} (\eta \cdot \eta)^n \eta_+^l |0\rangle. \quad (9.17)$$

To compare the two so as to get the phase factor we first note that

$$\eta_+ = \frac{1}{\sqrt{2}}(x_+ - ip_+) = \frac{1}{\sqrt{2}}\left(x_+ - \frac{\partial}{\partial x^+}\right) = \frac{1}{\sqrt{2}}\left(x_+ + \frac{\partial}{\partial x_-}\right), \quad (9.18)$$

then we use (9.16), (9.17) and the fact that $r^2 = -2x_+x_- + x_0^2$ so that $\partial f(r)/\partial x_- = -(x_+/r)\partial f/\partial r$; therefore we get

$$\begin{aligned} |nl+1l+1\rangle &= \frac{A_{nl+1}}{A_{nl}} \left[\frac{(2l+3)(2l+2)}{2} \right]^{\frac{1}{2}} \frac{1}{l+1} \eta_+ |nll\rangle \\ &= \frac{A_{nl+1}}{A_{nl}} \frac{[(2l+3)(2l+2)]^{\frac{1}{2}}}{2(l+1)} \left(x_+ + \frac{\partial}{\partial x_-} \right) |nll\rangle \\ &= \frac{A_{nl+1}}{A_{nl}} \left[\frac{(2l+3)!}{4\pi 2^l} \right]^{1/2} \frac{1}{(l+1)!} \sum_k [a_{nlk} - (k+1)a_{nlk+1}] r^{2k} e^{-\frac{1}{2}r^2} x_+^l \end{aligned} \quad \left. \right\} \quad (9.19)$$

Thus we obtain

$$a_{nl+10} = \frac{A_{nl+1}}{A_{nl}} \sqrt{2}(a_{nl0} - a_{nl1}), \quad (9.20)$$

where because of (1.9) the bracket is positive, implying that A_{nl+1} and A_{nl} have the same sign. As the reasoning can be repeated when we apply powers of the operator η_+ , it is clear that the phase factor is independent of l .

We now note that

$$\eta \cdot \eta = r^2 - \frac{1}{2}(p^2 + r^2) - \frac{3}{2} - i\mathbf{r} \cdot \mathbf{p} = r^2 - H_{ho} - \frac{3}{2} - \mathbf{r} \cdot \nabla, \quad (9.21)$$

so from (9.16) and (9.17) we get

$$\begin{aligned} |n+1l\rangle &= \frac{A_{n+1l}}{A_{nl}} (\eta \cdot \eta) |nl\rangle \\ &= \frac{A_{n+1l}}{A_{nl}} \sqrt{\left(\frac{(2l+1)!}{2^l 4\pi}\right)} \frac{1}{l!} \left(\frac{x_+}{r}\right)^l \\ &\sum_k [2a_{nlk-1} - (2n+2k+l+3)a_{nlk}] r^{2k+l} e^{-\frac{1}{2}r^2}. \end{aligned} \quad (9.22)$$

Thus we obtain

$$a_{n+1l0} = -\frac{A_{n+1l}}{A_{nl}} (2n+l+3)a_{nl0}, \quad (9.23)$$

implying that A_{n+1l} and A_{nl} have opposite sign.

Since by definition $A_{00} = 1$, we see from the above discussion that the phase factor in (9.15) becomes

$$e^{i\delta_{nl}} = (-1)^n. \quad (9.24)$$

This is the phase factor of (8.19).

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Chapter II

The Two-Body Problem

10 Transformation Brackets For Two-Particle Harmonic Oscillator States

In the previous chapter we discussed the one-body problem in terms of single-particle harmonic oscillator states. The most general two-body problem could be expanded in terms of a two-particle harmonic oscillator state of total angular momentum Λ and projection M which is written, in Dirac's full notation, as

$$\begin{aligned} \langle \mathbf{x}_1, \mathbf{x}_2 | n_1 l_1, n_2 l_2, \Lambda M \rangle &= [\psi_{n_1 l_1}(\mathbf{x}_1) \psi_{n_2 l_2}(\mathbf{x}_2)]_{\Lambda M} \\ &\equiv \sum_{m_1 m_2} (-1)^{l_1 - l_2 + M} \sqrt{2\Lambda + 1} \begin{pmatrix} l_1 & l_2 & \Lambda \\ m_1 & m_2 & -M \end{pmatrix} \\ &\quad \times \psi_{n_1 l_1 m_1}(\mathbf{x}_1) \psi_{n_2 l_2 m_2}(\mathbf{x}_2). \end{aligned} \quad (10.1)$$

In (10.1) the square bracket with suffixes ΛM is a shorthand notation for the coupling of the angular momenta l_1 and l_2 that we indicate explicitly on the last line. We shall differentiate the coordinates and momenta of the particles by an index $s = 1, 2$ leaving lower indices for components when needed, e.g. x_{is} .

The state (10.1) is quite convenient for the calculation of matrix elements of one-body operators such as the kinetic energy or the common potential for each particle, because these operators act either on $\psi_{n_1 l_1 m_1}(\mathbf{x}_1)$ or $\psi_{n_2 l_2 m_2}(\mathbf{x}_2)$.

However, it is not at all convenient for operators such as the interaction energy $V(|\mathbf{x}_1 - \mathbf{x}_2|)$ which is a function of the relative coordinate. It seems therefore of interest to expand the state (10.1) in terms of states depending

on the relative and centre-of-mass coordinates; we define these, and their corresponding momenta, for convenience, with a numerical coefficient of $1/\sqrt{2}$:

$$\left. \begin{aligned} \dot{\mathbf{x}}_1 &= \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2) & \dot{\mathbf{p}}_1 &= \frac{1}{\sqrt{2}}(\mathbf{p}_1 - \mathbf{p}_2) \\ \dot{\mathbf{x}}_2 &= \frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2) & \dot{\mathbf{p}}_2 &= \frac{1}{\sqrt{2}}(\mathbf{p}_1 + \mathbf{p}_2). \end{aligned} \right\}. \quad (10.2)$$

We stress again that all \mathbf{x}, \mathbf{p} will be the dimensionless ones of section 1. *The dotted and double dotted notations will be used here extensively for different systems of coordinates. They will never be associated with time derivatives.*

The two-particle state in the relative and centre-of-mass coordinate system is then given by

$$\langle \dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2 | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \dot{\Lambda} \dot{M} \rangle \equiv [\psi_{\dot{n}_1 \dot{l}_1}(\dot{\mathbf{x}}_1) \psi_{\dot{n}_2 \dot{l}_2}(\dot{\mathbf{x}}_2)]_{\dot{\Lambda} \dot{M}}. \quad (10.3)$$

We note that if we do not use the full Dirac notation, a confusion may arise between the kets in (10.1) and (10.3); we shall try to avoid it by having ordinary letters $n_s l_s$ in the ket when we deal with $\mathbf{x}_1, \mathbf{x}_2$ and dotted ones $\dot{n}_s \dot{l}_s$ when we deal with $\dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2$.

From (10.2) we note that

$$\begin{aligned} H &= \frac{1}{2}[(\mathbf{p}_1)^2 + (\mathbf{x}_1)^2 + (\mathbf{p}_2)^2 + (\mathbf{x}_2)^2] \\ &= \frac{1}{2}[(\dot{\mathbf{p}}_1)^2 + (\dot{\mathbf{x}}_1)^2 + (\dot{\mathbf{p}}_2)^2 + (\dot{\mathbf{x}}_2)^2] = \dot{H}, \end{aligned} \quad (10.4)$$

$$\begin{aligned} \mathbf{L} &= \mathbf{l}_1 + \mathbf{l}_2 = \mathbf{x}_1 \times \mathbf{p}_1 + \mathbf{x}_2 \times \mathbf{p}_2 = \dot{\mathbf{x}}_1 \times \dot{\mathbf{p}}_1 + \dot{\mathbf{x}}_2 \times \dot{\mathbf{p}}_2 \\ &= \dot{\mathbf{l}}_1 + \dot{\mathbf{l}}_2 = \dot{\mathbf{L}}, \end{aligned} \quad (10.5)$$

so that in expansion of states (10.1) in terms of those of (10.3) we must have $\Lambda = \dot{\Lambda}$, $M = \dot{M}$, and besides,

$$2\dot{n}_1 + \dot{l}_1 + 2\dot{n}_2 + \dot{l}_2 = 2n_1 + l_1 + 2n_2 + l_2. \quad (10.6)$$

The transformation brackets we are interested in are then those in the expansion

$$|n_1 l_1, n_2 l_2, \Lambda M\rangle = \sum_{\substack{\dot{n}_1 \dot{n}_2 \\ \dot{l}_1 \dot{l}_2}} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M\rangle \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda |n_1 l_1, n_2 l_2, \Lambda\rangle, \quad (10.7)$$

where the summation is finite because \dot{n}_s, \dot{l}_s are nonnegative integers restricted by (10.6) and the rule of addition of angular momenta:

$$|\dot{l}_1 - \dot{l}_2| \leq \Lambda \leq \dot{l}_1 + \dot{l}_2. \quad (10.8)$$

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The brackets are independent of M ; (10.5) shows that we could get states with $M + 1$ on both sides of Eq. (10.7) when we apply the operator

$$[(\Lambda - M)(\Lambda + M + 1)]^{-\frac{1}{2}}(L_1 + iL_2). \quad (10.9)$$

To derive the explicit form of the transformation brackets for harmonic oscillator states when we pass from the coordinates $\mathbf{x}_1, \mathbf{x}_2$ to $\dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2$ we shall start by expressing the two-particle state (10.1) in terms of creation operators. From section 8 we see that

$$\begin{aligned} &|n_1 l_1, n_2 l_2, \Lambda M\rangle \\ &= A_{n_1 l_1} A_{n_2 l_2} (\eta_1 \cdot \eta_1)^{n_1} (\eta_2 \cdot \eta_2)^{n_2} [\mathcal{Y}_{l_1}(\eta_1) \mathcal{Y}_{l_2}(\eta_2)]_{\Lambda M} |0\rangle, \end{aligned} \quad (10.10)$$

where

$$\eta_s \equiv \frac{1}{\sqrt{2}}(\mathbf{x}_s i \mathbf{p}_s), \quad s = 1, 2, \quad (10.11)$$

and

$$|0\rangle = \pi^{-\frac{3}{2}} \exp\{-\frac{1}{2}[(x_1)^2 + (x_2)^2]\} = \pi^{-\frac{3}{2}} \exp\{-\frac{1}{2}[(\dot{x}_1)^2 + (\dot{x}_2)^2]\}. \quad (10.12)$$

We will first obtain a relation for the transformation brackets for $n_1 = n_2 = 0$, and then derive a recursion relation which allows us to evaluate them for arbitrary n_1 and n_2 . For $n_1 = n_2 = 0$ (10.10) reduces to

$$|0 l_1, 0 l_2, \Lambda M\rangle = A_{0 l_1} A_{0 l_2} [\mathcal{Y}_{l_1}(\eta_1) \mathcal{Y}_{l_2}(\eta_2)]_{\Lambda M} |0\rangle. \quad (10.13)$$

From (10.2) the creation operators in the relative coordinate system are given by

$$\left. \begin{aligned} \dot{\eta}_1 &= \frac{1}{\sqrt{2}}(\eta_1 - \eta_2) \\ \dot{\eta}_2 &= \frac{1}{\sqrt{2}}(\eta_1 + \eta_2) \end{aligned} \right\}. \quad (10.14)$$

The procedure we follow will be to express (10.13) in terms of the $\dot{\eta}_1, \dot{\eta}_2$ and then compare this result with (10.3). First, however, we must discuss the meaning of $\mathcal{Y}_{lm}(\eta)$ as a function of $\dot{\eta}_1$ and $\dot{\eta}_2$ or (what is more convenient) to discuss an equivalent problem for ordinary coordinates, just as in section 8. Suppose we have a solid spherical harmonic $\mathcal{Y}_{lm}(r) = r^l Y_{lm}(\theta, \varphi)$ where

$$\mathbf{r} = \mathbf{r}' - \mathbf{r}'', \quad (10.15)$$

and we want to express $\mathcal{Y}_{lm}(\mathbf{r})$ as a function of \mathbf{r}' and \mathbf{r}'' . With \mathbf{r}'' fixed $\nabla^2 \mathcal{Y}_{lm} = (\nabla')^2 \mathcal{Y}_{lm} = 0$, for \mathbf{r} differs from \mathbf{r}' only by a translation. Similarly, $(\nabla'')^2 \mathcal{Y}_{lm} = 0$. Hence, the expansion must be in terms of the form

$$(r')^{l'} (r'')^{l''} [Y_{l'}(\theta', \varphi') Y_{l''}(\theta'', \varphi'')]_{lm} = [\mathcal{Y}_{l'}(\mathbf{r}') \mathcal{Y}_{l''}(\mathbf{r}'')]_{lm}. \quad (10.16)$$

Now \mathcal{Y}_{lm} is homogeneous of degree l in r , and thus also in r' and r'' , therefore,

$$l' + l'' = l. \quad (10.17)$$

A linear combination of (10.16) must equal \mathcal{Y}_{lm} :

$$\begin{aligned} \mathcal{Y}_{lm}(\mathbf{r}) &= r^l Y_{lm}(\theta, \varphi) \\ &= \sum_{l', l''=0}^l \delta_{l, l'+l''} G(l'l''l) (r')^{l'} (r'')^{l''} [Y_{l'}(\theta', \varphi') Y_{l''}(\theta'', \varphi'')]_{lm}, \end{aligned} \quad (10.18)$$

where $G(l'l''l)$ is a coefficient to be determined and $\delta_{l, l'+l''}$ is a Kronecker delta.

To evaluate G assume $\theta' = \theta'' = 0$; this implies $\theta = 0$ whence $r = r' - r''$. Using $Y_{lm}(0, 0) = [4\pi/(2l+1)]^{-\frac{1}{2}} \delta_{m0}$, (10.18) becomes

$$\begin{aligned} \left[\frac{4\pi}{2l+1} \right]^{-\frac{1}{2}} (r' - r'')^l &= \sum_{l', l''=0}^l \delta_{l, l'+l''} G(l'l''l) (-1)^{l'-l''} \begin{pmatrix} l' & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \\ &\times \left[\frac{(4\pi)^2}{(2l+1)(2l'+1)(2l''+1)} \right]^{-\frac{1}{2}} (r')^{l'} (r'')^{l''}. \end{aligned} \quad (10.19)$$

Expanding $(r' - r'')^l$ and using the closed form [1] of the $3j$ coefficient in (10.19), we get

$$G(l'l''l) = (-1)^{l''} \sqrt{\frac{(4\pi)(2l+1)!}{(2l'+1)!(2l''+1)!}}. \quad (10.20)$$

Let us return now to $|0l_1, 0l_2, \Lambda M\rangle$. We see that we can write for the spherical harmonic

$$\mathcal{Y}_{l_1 m_1}(\eta_1) = 2^{-\frac{1}{2} l_1} \sum_{l'_1, l'_2} (-1)^{l'_2} G(l'_1 l'_2 l_1) \delta_{l_1, l'_1 + l'_2} [\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_1 m_1}, \quad (10.21)$$

where the factor $2^{-\frac{1}{2} l_1}$ arises from the additional $\sqrt{2}$ in $\eta_1 = 2^{-\frac{1}{2}}(\dot{\eta}_1 + \dot{\eta}_2)$, whereas in (10.15) $\mathbf{r} = \mathbf{r}' - \mathbf{r}''$, and the $(-1)^{l'_2}$ comes from the change in sign

$$\mathcal{Y}_{lm}(-\mathbf{r}) = r^l Y_{lm}(\pi - \theta, \pi + \varphi) = (-1)^l r^l Y_{lm}(\theta, \varphi) = (-1)^l \mathcal{Y}_{lm}(\mathbf{r}).$$

Similarly,

$$\mathcal{Y}_{l_2 m_2}(\eta_2) = 2^{-\frac{1}{2} l_2} \sum_{l'_1 l'_2} (-1)^{l_2} G(l'_1 l'_2 l_2) \delta_{l_2, l'_1 + l'_2} [\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_2 m_2}. \quad (10.22)$$

We can now use $9j$ coefficients [2] to recouple the product

$$[[\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_1} [\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_2}]_{\Lambda M} \quad (10.23)$$

in terms of the product

$$[[\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_1} [\mathcal{Y}_{l'_2}(\dot{\eta}_2) \mathcal{Y}_{l'_1}(\dot{\eta}_1)]_{l_2}]_{\Lambda M}. \quad (10.24)$$

Furthermore we can expand the product of solid spherical harmonics in terms of ordinary spherical harmonics and powers of $(\eta \cdot \eta)^n$ by using the relation for the product of ordinary spherical harmonics [3]:

$$\begin{aligned} Y_{l'm'}(\theta, \varphi) Y_{l''m''}(\theta, \varphi) &= \sum_{lm} H(l'l''l) (-1)^{l'-l''+m} \\ &\times \sqrt{2l+1} \begin{pmatrix} l' & l'' & l \\ m' & m'' & -m \end{pmatrix} Y_{lm}(\theta, \varphi), \end{aligned} \quad (10.25)$$

where

$$H(l'l''l) = \sqrt{\frac{(2l'+1)(2l''+1)}{4\pi}} (-1)^{l'-l''} \begin{pmatrix} l' & l'' & l \\ 0 & 0 & 0 \end{pmatrix}. \quad (10.26)$$

With the help of the last equations we obtain, for example,

$$[\mathcal{Y}_{l'_1}(\dot{\eta}_1) \mathcal{Y}_{l'_2}(\dot{\eta}_2)]_{l_1 m_1} = \delta_{l'_1 + l'_2, 2\dot{\eta}_1 + l_1} H(l'_1 l'_2 l_1) (\dot{\eta}_1 \cdot \dot{\eta}_2)^{l_1} \mathcal{Y}_{l_1 m_1}(\dot{\eta}_1). \quad (10.27)$$

Combining all the previous results we see that the states (10.13) could be decomposed into states of relative and centre-of-mass coordinates as

$$|0l_1, 0l_2, \Lambda M\rangle = \sum_{\substack{\dot{\eta}_1 \dot{\eta}_2 \\ l_1 l_2}} |\dot{\eta}_1 l_1, \dot{\eta}_2 l_2, \Lambda M\rangle \langle \dot{\eta}_1 l_1, \dot{\eta}_2 l_2, \Lambda |0l_1, 0l_2, \Lambda\rangle, \quad (10.28)$$

where the coefficient

$$\langle \dot{\eta}_1 l_1, \dot{\eta}_2 l_2, \Lambda |0l_1, 0l_2, \Lambda\rangle \quad (10.29)$$

is given by

$$\begin{aligned} & \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | 0l_1, 0l_2, \Lambda \rangle \\ &= 2^{-\frac{1}{2}(l_1+l_2)} A_{0l_1} A_{0l_2} \sum_{\substack{\dot{l}'_1 \dot{l}'_2 \\ \dot{l}''_1 \dot{l}''_2}} \left[G(\dot{l}'_1 \dot{l}''_2 l_1) G(\dot{l}''_1 \dot{l}''_2 l_2) \delta_{l_1, \dot{l}'_1 + \dot{l}''_2} \delta_{l_2, \dot{l}'_2 + \dot{l}''_2} \right. \\ &\quad \times [(2l_1+1)(2l_2+1)(2\dot{l}_1+1)(2\dot{l}_2+1)]^{\frac{1}{2}} \\ &\quad \times \left\{ \begin{array}{ccc} \dot{l}'_1 & \dot{l}'_2 & l_1 \\ \dot{l}''_1 & \dot{l}''_2 & l_2 \\ l_1 & l_2 & \Lambda \end{array} \right\} \delta_{\dot{l}'_1 + \dot{l}''_1, 2\dot{n}_1 + \dot{l}_1} \\ &\quad \left. \times \delta_{\dot{l}'_2 + \dot{l}''_2, 2\dot{n}_2 + \dot{l}_2} H(\dot{l}'_1 \dot{l}''_1 l_1) H(\dot{l}''_2 \dot{l}'_2 l_2) A_{\dot{n}_1 \dot{l}_1}^{-1} A_{\dot{n}_2 \dot{l}_2}^{-1} \right]. \end{aligned} \quad (10.30)$$

In (10.30) $\{ \}$ stands for a $9j$ symbol and as there are four Kronecker deltas and summations over four variables, one might suppose that (10.30) reduces to a single term. However, one of the Kronecker deltas is redundant, for $l_1 + l_2 = \dot{l}'_1 + \dot{l}''_1 + \dot{l}'_2 + \dot{l}''_2 = 2\dot{n}_1 + \dot{l}_1 + 2\dot{n}_2 + \dot{l}_2 = \text{total energy}$. We are then left with one summation. A simplified expression for (10.30) is given in reference [4].

The general transformation bracket may be obtained from (10.30) with the help of recursion relations which we now derive. From our discussion in section 8 we know that

$$|n_1 + 1l_1, n_2 l_2, \Lambda M\rangle = \frac{A_{n_1+1l_1}}{A_{n_1 l_1}} (\eta_1 \cdot \eta_1) |n_1 l_1, n_2 l_2, \Lambda M\rangle. \quad (10.31)$$

Using (9.15) and (10.14) we get

$$\begin{aligned} & \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 + 1l_1, n_2 l_2, \Lambda \rangle \\ &= -2[(n_1 + l_1 + \frac{3}{2})(n_1 + 1)]^{\frac{1}{2}} \sum_{\substack{\dot{n}'_1 \dot{n}'_2 \\ \dot{l}'_1 \dot{l}'_2}} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | (\frac{1}{2}(\dot{\eta}_1 \cdot \dot{\eta}_1) \\ &\quad + \frac{1}{2}(\dot{\eta}_2 \cdot \dot{\eta}_2) + (\dot{\eta}_1 \cdot \dot{\eta}_2)) |\dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda \rangle \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle \\ &= \sum_{\substack{\dot{n}'_1 \dot{n}'_2 \\ \dot{l}'_1 \dot{l}'_2}} \frac{A_{n_1+1l_1}}{A_{n_1 l_1}} \left\{ \frac{1}{2} \frac{A_{\dot{n}'_1 \dot{l}'_1}}{A_{\dot{n}'_1 + 1 \dot{l}'_1}} \delta_{\dot{n}_1, \dot{n}'_1 + 1} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{n}'_2 \dot{n}_2} \delta_{\dot{l}'_2 \dot{l}_2} + \frac{1}{2} \frac{A_{\dot{n}'_2 \dot{l}'_2}}{A_{\dot{n}'_2 + 1 \dot{l}'_2}} \right. \\ &\quad \left. \delta_{\dot{n}'_1 \dot{n}_1} \delta_{\dot{n}'_2 + 1, \dot{n}_2} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{l}'_2 \dot{l}_2} + \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | \dot{\eta}_1 \cdot \dot{\eta}_2 | \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda \rangle \right\} \\ &\quad \times \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle. \end{aligned} \quad (10.32)$$

Finally from the well-known analysis of Racah [1] we get

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$$\begin{aligned} & \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | \dot{\eta}_1 \cdot \dot{\eta}_2 | \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda \rangle \\ &= (-1)^{l_2 + \dot{l}'_1 + \Lambda} \left\{ \begin{array}{ccc} \dot{l}_1 & \dot{l}_2 & \Lambda \\ \dot{l}'_2 & \dot{l}'_1 & 1 \end{array} \right\} \sqrt{(2\dot{l}_1 + 1)(2\dot{l}_2 + 1)} \\ &\quad \langle \dot{n}_1 \dot{l}_1 \| \dot{\eta}_1 \| \dot{n}'_1 \dot{l}'_1 \rangle \langle \dot{n}_2 \dot{l}_2 \| \dot{\eta}_2 \| \dot{n}'_2 \dot{l}'_2 \rangle, \end{aligned} \quad (10.33)$$

in which $\{ \}$ is a $6j$ symbol and where in turn the reduced matrix elements may be obtained by using

$$\begin{aligned} \eta_q |nlm\rangle &= \eta_q A_{nl} (\eta \cdot \eta)^n \mathcal{Y}_{lm}(\eta) |0\rangle \\ &= A_{nl} \sqrt{\frac{4\pi}{3}} (-1)^{l-1+m+q} \left\{ \frac{1}{A_{nl+1}} H(l1l+1) \sqrt{2l+3} \right. \\ &\quad \times \left(\begin{array}{ccc} l & 1 & l+1 \\ m & q & -m-q \end{array} \right) |nl+1m+q\rangle \\ &\quad + \frac{1}{A_{n+1l-1}} H(l1l-1) \sqrt{2l-1} \\ &\quad \left. \times \left(\begin{array}{ccc} l & 1 & l-1 \\ m & q & -m-q \end{array} \right) |n+1l-1m+q\rangle \right\}. \end{aligned} \quad (10.34)$$

Here the subindex $q = 1, 0, -1$ indicates the spherical components of the vector η .

Hence,

$$\begin{aligned} \langle n' l' \| \eta \| nl \rangle &= \sqrt{\frac{8\pi}{3}} \left\{ \sqrt{(n+l+\frac{3}{2})} H(l1l+1) \delta_{n'n} \delta_{l'l+1} \right. \\ &\quad \left. - \sqrt{(n+1)} H(l1l-1) \delta_{n'n+1} \delta_{l'l-1} \right\}. \end{aligned} \quad (10.35)$$

Combining all of these results, we get

$$\begin{aligned} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 + 1l_1, n_2 l_2, \Lambda \rangle &= [(n_1 + 1)(n_1 + l_1 + \frac{3}{2})]^{-\frac{1}{2}} \\ &\quad \times \sum_{\substack{\dot{n}'_1 \dot{n}'_2 \\ \dot{l}'_1 \dot{l}'_2}} M(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2; \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda) \\ &\quad \times \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle, \end{aligned} \quad (10.36)$$

where the coefficient $M(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2; \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda)$ may be calculated from (10.32) and (10.33). The summation will be greatly limited by the Kronecker deltas appearing in (10.32) and (10.35). There are, in fact, only six nonzero matrix elements, which are listed in Table II.1.

Table II.1. Matrix needed in the recurrence relations of the transformation brackets for arbitrary n_1 and n_2 . The symbol $\{ \}$ stands for a $6j$ coefficient.

n'_1	l'_1	n'_2	l'_2	$M(n_1 l_1, n_2 l_2; n'_1 l'_1, n'_2 l'_2, \Lambda)$
$n_1 - 1$	l_1	n_2	l_2	$\frac{1}{2}[n_1(n_1 + l_1 + \frac{1}{2})]^{1/2}$
n_1	l_1	$n_2 - 1$	l_2	$\frac{1}{2}[n_2(n_2 + l_2 + \frac{1}{2})]^{1/2}$
$n_1 - 1$	$l_1 + 1$	$n_2 - 1$	$l_2 + 1$	$[n_1 n_2(l_1 + 1)(l_2 + 1)]^{\frac{1}{2}}(-1)^{l_1 + l_2 + \Lambda} \left\{ \begin{array}{c} l_1 \\ l_2 + 1 \\ l_1 + 1 \\ l_2 \\ l_1 \\ \Lambda \end{array} \right\}$
$n_1 - 1$	$l_1 + 1$	n_2	$l_2 - 1$	$[n_1(n_2 + l_2 + \frac{1}{2})(l_1 + 1)l_2]^{\frac{1}{2}}(-1)^{l_1 + l_2 + \Lambda} \left\{ \begin{array}{c} l_1 \\ l_2 - 1 \\ l_1 + 1 \\ l_2 \\ l_1 \\ \Lambda \end{array} \right\}$
n_1	$l_1 - 1$	$n_2 - 1$	$l_2 + 1$	$[(n_1 + l_1 + \frac{1}{2})n_2 l_1(l_2 + 1)]^{\frac{1}{2}}(-1)^{l_1 + l_2 + \Lambda} \left\{ \begin{array}{c} l_1 \\ l_2 + 1 \\ l_1 - 1 \\ l_2 \\ l_1 \\ \Lambda \end{array} \right\}$
n_1	$l_1 - 1$	n_2	$l_2 - 1$	$[(n_1 + l_1 + \frac{1}{2})(n_2 + l_2 + \frac{1}{2})l_1 l_2]^{\frac{1}{2}}(-1)^{l_1 + l_2 + \Lambda} \left\{ \begin{array}{c} l_1 \\ l_2 - 1 \\ l_1 - 1 \\ l_2 \\ l_1 \\ \Lambda \end{array} \right\}$

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The transformation bracket

$$\langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 + 1 l_2, \Lambda \rangle \quad (10.37)$$

may be evaluated in a similar manner. We would obtain a formula similar to (10.36), but with the indices of the first factor changed from 1 to 2. The table for the matrix element M will be the same as Table II.1, but the last four lines will have their signs changed.

By means of the recursion relation for n_1 (10.36), and a similar one for n_2 , we may express the transformation brackets with arbitrary n_1 and n_2 in terms of the transformation brackets for $n_1 - 1$ and n_2 , etc. We may thus obtain the transformation brackets for arbitrary n_1 and n_2 in terms of the bracket with $n_1 = n_2 = 0$, for which we already have an explicit expression in (10.30).

Computer programs are available for the transformation brackets using the analysis developed in this section. Tables have also been published in reference [4]. When making use of these tables it is convenient to keep in mind some of the symmetry relations for the transformation brackets derived in reference [5]:

$$\begin{aligned} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle &= (-1)^{l_2 - \Lambda} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_2 l_2, n_1 l_1, \Lambda \rangle \\ &= (-1)^{l_1 - \Lambda} \langle \dot{n}_2 \dot{l}_2, \dot{n}_1 \dot{l}_1, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle \\ &= (-1)^{l_1 + l_2} \langle \dot{n}_2 \dot{l}_2, \dot{n}_1 \dot{l}_1, \Lambda | n_2 l_2, n_1 l_1, \Lambda \rangle \\ &= (-1)^{l_2 + \Lambda} \langle n_1 l_1, n_2 l_2, \Lambda | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda \rangle. \end{aligned} \quad (10.38)$$

Other computer programs for the transformation brackets have been developed by Baranger and Davies [6], using recurrence relations in l_1, l_2 for given n_1, n_2 . These have proved useful in some of the Hartree-Fock calculations discussed in Chapter V.

It is very important to notice that the transformation brackets defined in (10.7) connect two kets associated respectively with the coordinates x_1, x_2 and \dot{x}_1, \dot{x}_2 . If instead of the kets we had two bras $\langle n_1 l_1, n_2 l_2, \Lambda M |$ and $\langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M |$, the relation corresponding to (10.7) becomes

$$\begin{aligned} \langle n_1 l_1, n_2 l_2, \Lambda M | &= \sum_{i_1 i_2} \langle n_1 l_1, n_2 l_2, \Lambda | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda \rangle \\ &\quad \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M |, \end{aligned} \quad (10.39)$$

where we use round parentheses for the transformation brackets to distinguish them from the angular ones appearing in (10.7).

If we take the transposed conjugate of both sides of (10.39) and make use of the standard relation between bras and kets, as well as of the fact

that the transformation brackets derived in this section are real numbers, we obtain

$$\langle n_1 l_1, n_2 l_2, \Lambda | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda \rangle = \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle. \quad (10.40)$$

When we calculate matrix elements with respect to the states of coordinates $\mathbf{x}_1, \mathbf{x}_2$ and transform them to matrix elements for states with coordinates $\dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2$, we get both transformation brackets, $\langle \rangle$ from the ket and $\langle \rangle$ from the bra. Since the published tables [4] give only the $\langle \rangle$ brackets, we use in all that follows the relation (10.40) in order to express the matrix elements entirely in terms of these brackets.

11 Applications of the Transformation Brackets to Atomic Problems. The Helium Atom

As an illustration of the application of the transformation brackets in atomic physics, we shall discuss their use in a two-electron problem such as the helium atom.

In terms of the dimensionless variables of section 3, the Hamiltonian of the He atom is given by

$$H = \frac{1}{2}\epsilon^2[(\mathbf{p}_1)^2 + (\mathbf{p}_2)^2] + \sqrt{2}\epsilon \left[\frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} - \frac{2}{|\mathbf{x}_1|} - \frac{2}{|\mathbf{x}_2|} \right]. \quad (11.1)$$

The integrals of motion of this Hamiltonian obviously include the square of the total angular momentum, L^2 , its projection L_3 and the parity, as well as the operator of permutation of particles 1 and 2. The eigenfunctions of H can then be expanded in terms of the two-particle harmonic oscillator states

$$\begin{aligned} |n_1 l_1, n_2 l_2, \Lambda M\rangle_{S,A} &\equiv \frac{1}{\sqrt{2}} \left[|n_1 l_1, n_2 l_2, \Lambda M\rangle \right. \\ &\quad \left. \pm (-1)^{l_1+l_2-\Lambda} |n_2 l_2, n_1 l_1, \Lambda M\rangle \right], \end{aligned} \quad (11.2)$$

with either the + or - sign depending on whether the states are symmetric (S) or antisymmetric (A) under interchange of particles 1 and 2. States of positive (negative) parity can only be expanded in terms of those of the type (11.2) with total number of quanta $2n_1 + l_1 + 2n_2 + l_2$ even (odd). We have assumed in (11.2) that the two electrons do not occupy the same orbital, i.e., $(n_1, l_1) \neq (n_2, l_2)$; if they do, we must include an additional

factor $1/\sqrt{2}$ in the normalization, for then there are only symmetric states for Λ even and antisymmetric for Λ odd.

By the same reasoning as in section 3, a variational analysis of the energy of the He atom leads to the diagonalization of the matrix of the Hamiltonian

$$\|_{S,A} \langle n'_1 l'_1, n'_2 l'_2, \Lambda M | H | n_1 l_1, n_2 l_2, \Lambda M \rangle_{S,A} \| . \quad (11.3)$$

In (11.3) Λ and the symmetry character of the harmonic oscillator states are fixed, and $n_1 l_1 n_2 l_2$ take all possible nonnegative integer values consistent with Λ , parity and with

$$2n_1 + l_1, 2n_2 + l_2 \leq \mathfrak{N}, \quad (11.4)$$

where \mathfrak{N} is the maximum number of quanta we shall consider in the approximation.

From (11.1) we see that the matrix elements in (11.3) can be expressed as sums of terms of the type

$$\begin{aligned} &\langle n'_1 l'_1, n'_2 l'_2, \Lambda M | \frac{1}{2}\epsilon^2(\mathbf{p}_1)^2 - \sqrt{2}\epsilon \frac{2}{|\mathbf{x}_1|} | n_1 l_1, n_2 l_2, \Lambda M \rangle \\ &= \delta_{n'_2 n_2} \delta_{l'_2 l_2} \delta_{l'_1 l_1} \langle n'_1 l_1 m_1 | \frac{1}{2}\epsilon^2(\mathbf{p}_1)^2 - \sqrt{2}\epsilon \frac{2}{|\mathbf{x}_1|} | n_1 l_1 m_1 \rangle \end{aligned} \quad (11.5)$$

(where the last matrix element is independent of m_1 , as was fully discussed in section 3) and the matrix element

$$\langle n'_1 l'_1, n'_2 l'_2, \Lambda M | \frac{\sqrt{2}\epsilon}{|\mathbf{x}_1 - \mathbf{x}_2|} | n_1 l_1, n_2 l_2, \Lambda M \rangle. \quad (11.6)$$

For the latter we may use (10.2) and the transformation brackets of section 10 together with the matrix elements of section 3, to write

$$\begin{aligned} &\langle n'_1 l'_1, n'_2 l'_2, \Lambda M | \frac{\epsilon}{|\dot{\mathbf{x}}_1|} | n_1 l_1, n_2 l_2, \Lambda M \rangle \\ &= \epsilon \sum_{\substack{n'_1 l_1 n_2 \\ l_1 l_2}} \sum_p \langle \dot{n}'_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n'_1 l'_1, n'_2 l'_2, \Lambda \rangle \\ &\quad \times B(\dot{n}'_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, p) \frac{p!}{\Gamma(p + \frac{3}{2})} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle. \end{aligned} \quad (11.7)$$

Thus the explicit form of the matrix elements in (11.3) can be written down immediately.

Returning then to the problem of the helium atom, we see that for $\mathfrak{N} = 0$ we have just one matrix element:

$$E(\epsilon) \equiv \langle 00, 00, 0 | H | 00, 00, 0 \rangle = \frac{3}{2}\epsilon^2 - 8\epsilon\sqrt{\frac{2}{\pi}} + \frac{2\epsilon}{\sqrt{\pi}}. \quad (11.8)$$

Minimizing it with respect to ϵ we get

$$\epsilon = \frac{1}{3} \left(8\sqrt{\frac{2}{\pi}} - \frac{2}{\sqrt{\pi}} \right), \quad (11.9)$$

and the value of corresponding $E(\epsilon)$ is 79% of the experimental one.

For $\mathfrak{N} = 2$ we have the three states

$$\begin{aligned} &|00, 00, 00\rangle, \\ &\frac{1}{\sqrt{2}}(|10, 00, 00\rangle + |00, 10, 00\rangle), \\ &|01, 01, 00\rangle, \end{aligned} \quad \left. \right\}. \quad (11.10)$$

Diagonalizing the corresponding matrix and minimizing with respect to ϵ the value of the energy improves only to 80% of the experimental value. This is not unexpected, since we saw in section 3 that for the hydrogen atom the accuracy in the approximation increased appreciably only when steps of four quanta were taken rather than two. An analysis by Dubovoy [7] for the helium atom, using a maximum $\mathfrak{N} = 4$, yields a calculated energy for the ground state which is 92% of the experimental value.

12 Applications of the Transformation Brackets to Molecular Problems. The H_2 and H_3^+ Molecules

The Hamiltonian of a two-electron molecular problem is

$$H = \frac{1}{2}\epsilon^2[(p_1)^2 + (p_2)^2] + \sqrt{2}\epsilon \left[\frac{1}{|\mathbf{x}_1 - \mathbf{x}_2|} - \sum_{\alpha} \frac{Z_{\alpha}}{|\mathbf{x}_1 - \mathbf{X}_{\alpha}|} \right. \\ \left. - \sum_{\alpha} \frac{Z_{\alpha}}{|\mathbf{x}_2 - \mathbf{X}_{\alpha}|} + \sum_{\alpha < \beta} \frac{Z_{\alpha}Z_{\beta}}{|\mathbf{X}_{\alpha} - \mathbf{X}_{\beta}|} \right], \quad (12.1)$$

with Z_{α} , \mathbf{X}_{α} being respectively the charge and the position vector of the different nuclei. A variational calculation implies the diagonalization of the matrix of the operator H with respect to the states (11.2). The only matrix elements not fully discussed in section 11 are those of the type $|\mathbf{x}_1 - \mathbf{X}_{\alpha}|^{-1}$. Using the expansion of $|\mathbf{x}_1 - \mathbf{X}_{\alpha}|^{-1}$ given in (4.2), these matrix elements reduce to linear combinations of [1]

$$\begin{aligned} &\left\langle n'_1 l'_1, n'_2 l'_2, \Lambda' M' \left| \begin{bmatrix} r_1^k / R_{\alpha}^{k+1} \\ R_{\alpha}^k / r_1^{k+1} \end{bmatrix} Y_{kq}(\theta_1, \varphi_1) \right| n_1 l_1, n_2 l_2, \Lambda M \right\rangle \\ &= \delta_{n'_1 n_2} \delta_{l'_1 l_2} (-1)^{l_2 + l'_1 + M'} [(2l'_1 + 1)(2\Lambda + 1)(2\Lambda' + 1)]^{\frac{1}{2}} \\ &\times \left\{ \begin{array}{ccc} l_1 & \Lambda & l_2 \\ \Lambda' & l'_1 & k \end{array} \right\} \left(\begin{array}{ccc} \Lambda & k & \Lambda' \\ M & q & -M' \end{array} \right) \\ &\times \left\langle n'_1 l'_1 \left| \begin{bmatrix} r_1^k / R_{\alpha}^{k+1} \\ R_{\alpha}^k / r_1^{k+1} \end{bmatrix} Y_{kq}(\theta_1, \varphi_1) \right| n_1 l_1 \right\rangle, \end{aligned} \quad (12.2)$$

where $\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \end{array} \right\}$ is a $6j$ coefficient and the last term is the reduced matrix element given in (4.3). Note that in the molecular problem the operators of permutation of the coordinates are still integrals of motion, but the total angular momentum is not, so Λ is not a good quantum number. By the same reasoning M is a good quantum number only for linear molecules with nuclei along the z -axis, while the parity is an integral of motion only for nuclear configurations invariant under inversion.

Let us now consider the H_2 molecule where $\mathbf{X}_1 = \mathbf{X}$, $\mathbf{X}_2 = -\mathbf{X}$ and \mathbf{X} , of magnitude R , is taken along the z -axis. For the case $\mathfrak{N} = 0$ we see from sections 4 and 11 that

$$\langle 00, 00, 0 | H | 00, 00, 0 \rangle = \frac{3}{2}\epsilon^2 + \epsilon f(R), \quad (12.3)$$

where

$$f(R) = \frac{2}{\sqrt{\pi}} + \frac{1}{R\sqrt{2}}[1 - 8 \operatorname{erf}(R)]. \quad (12.4)$$

Minimizing with respect to ϵ, R (as in section 4), we get

$$\langle H \rangle_{\min} \equiv E(R) = \frac{1}{6}f(R_0)[f(R_0) - 2f(R)], \quad (12.5)$$

where R_0 is the value of R for which $f(R)$ of (12.4) is minimal.

The graph of $E(R)$ as function of R is given in Fig. II.1. For comparison we give the Heitler-London LCAO [8] curve, which has three parameters rather than the single parameter ϵ of the present analysis. The binding energy we get at the value of R that gives the minimum of $E(R)$ is 79% of the experimental value. The theoretical internuclear distance is $2R = 0.82$ Å against the experimental one 0.74 Å.

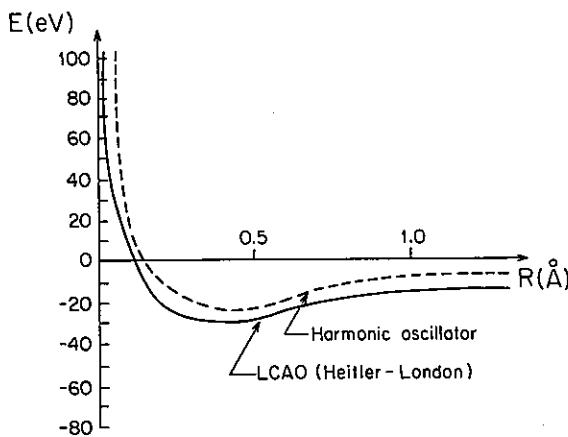


Figure II.1. Expectation value $E(R)$ of the Hamiltonian of the H_2 molecule as a function of R , half the internuclear distance. The two-electron wave function is represented by a zero-quantum state of the harmonic oscillator, whose frequency is chosen so as to minimize the energy $E(R)$. Here R is in Å, while in the text it is dimensionless.

When we extend our calculations to $\mathfrak{N} = 2$ we note that since we have a linear molecular with origin at the centre of charge, the states (11.2) must still have $M = 0$, positive parity and be symmetric under exchange of particles 1, 2. This implies then that besides the three states (11.10) we must consider

$$\frac{1}{\sqrt{2}} \left(|02, 00, 20\rangle + |00, 02, 20\rangle \right), \quad \text{and} \quad |01, 01, 20\rangle. \quad (12.6)$$

Taking for R the value $R = 0.41$ Å of the $\mathfrak{N} = 0$ approximation, and minimizing numerically the lowest eigenvalue of the 5×5 matrix with respect to ϵ we get an energy which is 84% of the experimental value.

As a final example we discuss the molecule H_3^+ , which has two electrons and three protons. It seems reasonable to assume, from symmetry considerations, that the three protons are either in an equally spaced linear chain, which can be taken as the z -axis of our reference frame, or at the vertices of an equilateral triangle. In both cases the origin of our coordinate system is taken at the centre of nuclear charge, as shown in Fig. II.2.

Let us start our analysis with the case $\mathfrak{N} = 0$, where a calculation entirely similar to the previous one for H_2 leads to

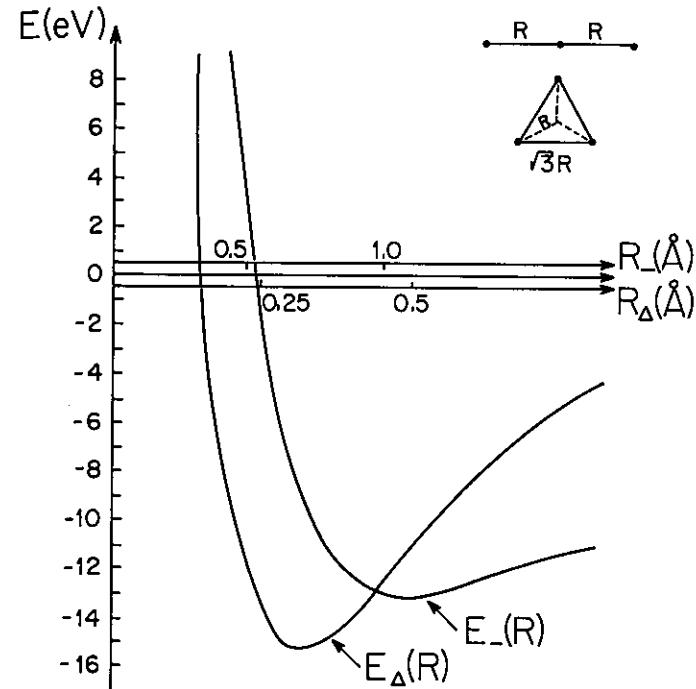


Figure II.2. Expectation values of the Hamiltonian of the H_3^+ molecule with respect to a two-electron wave function, when the latter is represented by a zero-quantum state of the harmonic oscillator. Two configurations for the three protons in the molecule are chosen, the linear chain and the equilateral triangle, and their energies are indicated by $E_-(R)$ and $E_\Delta(R)$ respectively, with the meaning of R in each case being indicated in the figure. As in the other problems the frequency is chosen to give a minimum for the energy.

$$\text{Triangular: } \langle H \rangle = \frac{3}{2} \epsilon^2 + \epsilon f_\Delta(R), \quad (12.7)$$

$$\text{Linear: } \langle H \rangle = \frac{3}{2} \epsilon^2 + \epsilon f_-(R), \quad (12.8)$$

where f_Δ and f_- are given by

$$f_\Delta(R) = -\frac{1}{R} 6\sqrt{2} \operatorname{erf}(R) + \frac{2}{\sqrt{\pi}} + \frac{\sqrt{6}}{R}, \quad (12.9)$$

$$f_-(R) = -\frac{1}{R} 4\sqrt{2} \operatorname{erf}(R) - 4\sqrt{\frac{2}{\pi}} + \frac{2}{\sqrt{\pi}} + \frac{5}{R\sqrt{2}}. \quad (12.10)$$

Minimizing $\langle H \rangle$ with respect to ϵ, R we arrive again at the expression (12.5) for $E(R)$, only instead of $f(R)$ we have $f_\Delta(R)$ or $f_-(R)$, depending

on whether the molecule is triangular or linear. The energies $E_{\Delta}(R)$, $E_{-}(R)$ are given in Fig. II.2, where we see that in the $\mathfrak{N} = 0$ approximation the triangular shape is more stable, *i.e.*, the minimum comes lower. The total energy at the minimum $E_{\Delta}(R_0) = -30.5$ eV, and the internuclear distance (see Fig. II.2) is $\sqrt{3}R = 0.845$ Å. Within our approximation H_3^+ is stable under disintegration into $H_2 + H^+$.

The calculations have been extended to $\mathfrak{N} = 2$, where the binding energy increases to -31.86 eV.

13 Matrix Elements in $j-j$ Coupling

In the previous sections of this chapter we calculated the matrix elements, with respect to two-particle harmonic oscillator states, of operators that were functions only of the coordinates and momenta of the particles. This was sufficient for the atomic and molecular problems, in which we disregard the effect of spin dependent forces. In the nuclear case both one- and two-body operators are usually spin-dependent, and so it frequently proves convenient to start with single-particle states in which the orbital and spin angular momentum are coupled to a total j . We will then need to calculate the matrix elements of one- and two-body operators with respect to two-particle states of this type. We shall discuss the evaluation of these matrix elements in the present section, and in particular derive convenient algebraic formulae, tabulated by Mavromatis *et al.* [9], which greatly simplify the calculations.

The single-nucleon wave function in $j-j$ coupling will be written as

$$\phi_{nljm} \equiv R_{nl}(r)[Y_l(\theta, \varphi)\chi_{\frac{1}{2}}]_{jm}, \quad (13.1)$$

where $\chi_{\frac{1}{2}m_s}$, $m_s = \pm \frac{1}{2}$, is the wave function of spin. The antisymmetric two-nucleon wave function is

$$\begin{aligned} & |n_1l_1j_1, n_2l_2j_2, JT\rangle_A \\ &= \frac{1}{\sqrt{2}} \left[|n_1l_1j_1, n_2l_2j_2, JT\rangle \right. \\ &\quad \left. + (-1)^{T+j_1+j_2-J} |n_2l_2j_2, n_1l_1j_1, JT\rangle \right], \end{aligned} \quad (13.2)$$

where

$$|n_1l_1j_1, n_2l_2j_2, JT\rangle = [\phi_{n_1l_1j_1}(1)\phi_{n_2l_2j_2}(2)]_{JM} [\tau_{\frac{1}{2}}(1)\tau_{\frac{1}{2}}(2)]_{TM_T}. \quad (13.3)$$

Here $\tau_{\frac{1}{2}m_i}(i)$, $i = 1, 2$, is the isospin function of the two particles corresponding to $\chi_{\frac{1}{2}m_s}(i)$, $i = 1, 2$, in the spin case, and TM_T are the total

isospin and its projection. In (13.2) we have explicitly assumed that the two nucleons are not in identical orbitals; to be strictly correct, we should multiply (13.2) by $[1 + \delta_{n_1n_2}\delta_{l_1l_2}]^{-\frac{1}{2}}$. We shall henceforth drop this factor.

To obtain the matrix elements, we first transform the states (13.2) to $L-S$ coupling:

$$|n_1l_1j_1, n_2l_2j_2, JT\rangle = \sum_{AS} |n_1l_1, n_2l_2, \Lambda; S; JT\rangle \begin{pmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ \Lambda & S & J \end{pmatrix}, \quad (13.4)$$

where the last term is related to a $9j$ coefficient by

$$\begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = [(2c+1)(2f+1)(2g+1)(2h+1)]^{\frac{1}{2}} \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}. \quad (13.5)$$

We then express the ket in the expansion (13.4) in terms of the relative and centre-of-mass coordinates:

$$|n_1l_1, n_2l_2, \Lambda; S; JT\rangle = \sum_{nlNL} |nl, NL, \Lambda; S; JT\rangle \langle nl, NL, \Lambda | n_1l_1, n_2l_2, \Lambda \rangle. \quad (13.6)$$

The transformation brackets in (13.6) are exactly those derived in section 10, though in a notation more familiar in the literature [4,9], with nLN replacing $n_1l_1n_2l_2$. We then transform the ket on the right-hand side of (13.6) by recoupling the relative angular momentum with the total spin:

$$\begin{aligned} & |nl, NL, \Lambda; S; JT\rangle = \sum_j |nlS(j), NL, JT\rangle \langle lS(j)LJ | LL(\Lambda)SJ \rangle \\ &= \sum_j |nlS(j), NL, JT\rangle [(2\Lambda+1)(2j+1)]^{\frac{1}{2}} \\ &\quad \times (-1)^{j+L+S+\Lambda} \begin{Bmatrix} j & L & J \\ \Lambda & S & l \end{Bmatrix}, \end{aligned} \quad (13.7)$$

where, as before, $\begin{Bmatrix} a & b & c \\ d & e & f \end{Bmatrix}$ is a $6j$ coefficient [1] and

$$|nlS(j), NL, JT\rangle = [[nlS(j), T\rangle | NL\rangle]_J, \quad (13.8)$$

with square bracket indicating vector coupling. In (13.8) the kets are in turn given by

$$|NLM\rangle = \langle \dot{x}_2 | NLM \rangle \quad (13.9a)$$

$$|nlS(j), T\rangle = [\langle \dot{x}_1 | nl \rangle [\chi_{\frac{1}{2}}(1)\chi_{\frac{1}{2}}(2)]_S]_J [\tau_{\frac{1}{2}}(1)\tau_{\frac{1}{2}}(2)]_T, \quad (13.9b)$$

where $j = l + S$.

Combining (13.4), (13.6) and (13.7), we obtain [9]

$$\begin{aligned} {}_A\langle n_1l_1j_1, n_2l_2j_2, JT | V | n_3l_3j_3, n_4l_4j_4, JT \rangle_A \\ = \sum_{\Lambda\Lambda'S} \begin{pmatrix} l_1 & \frac{1}{2} & j_1 \\ l_2 & \frac{1}{2} & j_2 \\ \Lambda & S & J \end{pmatrix} \begin{pmatrix} l_3 & \frac{1}{2} & j_3 \\ l_4 & \frac{1}{2} & j_4 \\ \Lambda' & S & J \end{pmatrix} \\ \times \sum_{\substack{n'l'l' \\ NL}} \langle nl, NL, \Lambda | n_1l_1, n_2l_2, \Lambda \rangle \\ \times \langle n'l', NL, \Lambda' | n_3l_3, n_4l_4, \Lambda' \rangle (-1)^{\Lambda+\Lambda'} [1 - (-1)^{l+S+T}] \\ \times \sum_j U(LlJS; \Lambda j) U(L'l'JS; \Lambda' j) \\ \times \langle nlS(j), T | V | n'l'S(j), T \rangle, \end{aligned} \quad (13.10)$$

where

$$U(abcd; ef) = [(2e+1)(2f+1)]^{\frac{1}{2}} (-1)^{a+b+c+d} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix}, \quad (13.11)$$

and the last matrix element is the one of the interaction potential with respect to the state (13.9b). The coefficients of this matrix element in (13.10) have been tabulated by Mavromatis, Sanderson and Singh [9].

Note that (13.9b) depends only on the single relative coordinate \mathbf{x}_1 , and so the last matrix element in (13.10) may be evaluated by a simple generalization of the analysis of section 2. The effect of a transposition (1,2) on the ket (13.8) is to multiply the relative coordinate part by $(-1)^l$ and the spin and isospin parts by $(-1)^{1-S}$ and $(-1)^{1-T}$ respectively. Thus the total effect of (1,2) on the kets is to introduce a factor $(-1)^{l+S+T}$, and so the term $\frac{1}{2}[1 - (-1)^{l+S+T}]$ in (13.10) guarantees the antisymmetry of the state, indicated by the subscripts A, A on the left-hand side of (13.10).

14 Application to Two-Particle Problems in the 2s-1d Nuclear Shell.

The ^{18}O and ^{18}F Nuclei

We have seen in (13.10) that the matrix element of a two-body interaction with respect to the two-particle state (13.2) reduces to sums of products of geometrical factors with the matrix elements

$$\langle nlS(j), T | V | n'l'S(j), T \rangle. \quad (14.1)$$

Before starting on the applications of (13.10) in nuclear physics, we shall discuss the evaluation of the matrix element (14.1) for particular types of forces.

If we have just a central force $V(r)$, the matrix elements reduces to

$$\langle n'l' | V(r) | nl \rangle = \delta_{ll'} \int_0^\infty R_{n'l'}(r) V(r) R_{nl}(r) r^2 dr, \quad (14.2)$$

where the integral is evaluated as in (2.3) and (2.5).

For a Majorana force $V(r)P^M$, where P^M is the Majorana projection operator, we have the same result as Eq. (14.2) multiplied by $(-1)^l$.

For a Bartlett force $V(r)P^B$, where P^B is the Bartlett projection operator, whose effect is the same as $S^2 - 1$, with S being the spin of the two particles, we have

$$\delta_{ll'} [S(S+1) - 1] \langle n'l' | V(r) | nl \rangle. \quad (14.3)$$

For a Heisenberg force, where the effect of the corresponding projection operator is that of $-(T^2 - 1)$ with T being the isospin of the two particles, we shall get a matrix element of the form (14.3) with T replacing S , and of the opposite sign.

The matrix element for a spin-orbit interaction $V(r)\mathbf{l} \cdot \mathbf{S}$ is easily obtained by writing $\mathbf{l} \cdot \mathbf{S} = \frac{1}{2}[j^2 - l^2 - S^2]$, thus getting

$$\frac{1}{2}[j(j+1) - l(l+1) - S(S+1)] \langle n'l' | V | nl \rangle \delta_{ll'}. \quad (14.4)$$

The tensor force may be put in the form [4]

$$V_T = \sqrt{\left(\frac{32\pi}{5}\right)} V(r) \mathbf{Y}_2(\theta, \varphi) \cdot \mathbf{X}_2. \quad (14.5)$$

Here \mathbf{Y}_2 is the Racah tensor with components $Y_{2m}(\theta, \varphi)$, r, θ and φ refer to the relative coordinates, and \mathbf{X}_2 is a second-order Racah tensor whose zero-component is given by

$$X_{20} = \frac{1}{\sqrt{2}} (3S_0^2 - S^2). \quad (14.6)$$

The matrix elements of the tensor force can then be easily evaluated using standard Racah algebra [4].

In this way we have evaluated the matrix elements of any type of interaction. One simple illustration may be taken from the calculation of energy levels in the 2s-1d nuclear shell [10]. Let us take, for instance, the cases of ^{18}O or ^{18}F . We recall that in the harmonic oscillator shell model we

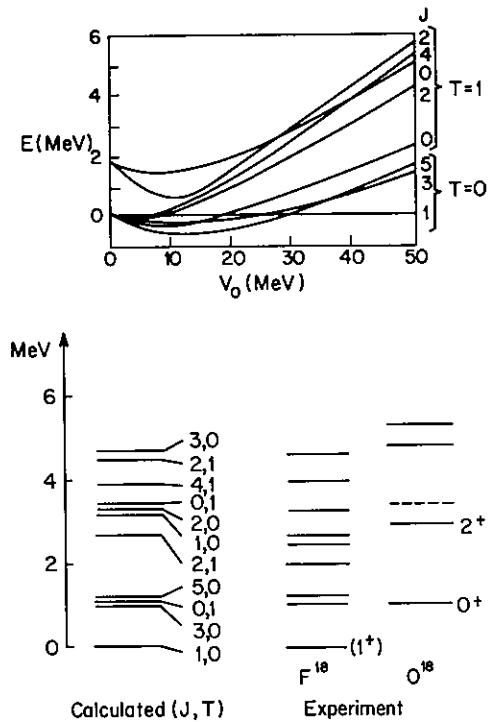


Figure II.3. (a) Calculated spectrum for nuclei with $A = 18$ plotted against the strength of the central force V_0 for fixed one-body forces such as the spin-orbit coupling. (b) Comparison of the experimental spectrum of $A = 18$ nuclei with theory for $V_0 = 42$ MeV. These figures were taken from J. P. Elliott and B. H. Flowers, reference [10].

may put 4 particles (2 neutrons and 2 protons) in the $1s$ shell; 12 particles (6 neutrons and 6 protons) in the $1p$ shell. Thus the ^{16}O corresponds to a closed shell and will be considered as a stable core in our analysis (we do not know of any excited states of ^{16}O below 6 MeV).

Thus ^{18}O and ^{18}F reduce to a problem of two particles in the $2s-1d$ shell in a potential well provided by the core. For these two nuclei we may therefore write the Hamiltonian as follows:

$$H = H_{\text{ho}} - \frac{\xi}{\hbar^2} \sum_{t=1}^2 \mathbf{l}_t \cdot \mathbf{s}_t - U_0 \sum_{t=1}^2 (\mathbf{l}_t)^2 + \frac{1}{3} V_0 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 [0.3 + 0.7 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2] e^{-r_{12}/a}. \quad (14.7)$$

Some comments about this Hamiltonian are in order. The term H_{ho} refers to the common harmonic oscillator potential. To account for the energy-level shifts in ^{17}O a spin-orbit coupling term is added as well as the term

$\sum (\mathbf{l}_t)^2$. The parameter ξ that appears in the spin-orbit term is obtained from the separation between the $d_{3/2}$ and $d_{5/2}$ levels in ^{17}O . It is found to be of the order of $\xi = 2$ MeV. The parameter U_0 is similarly determined from the separation of the $s_{1/2}$ and $d_{5/2}$ levels in ^{17}O . The last term in the Hamiltonian refers to the residual nucleon-nucleon interaction between each pair of particles in the $2s-1d$ shell, and was chosen to be a Rosenfeld force mixture. In this term the value of a was taken [10] as $a = 1.37$ fm, and $\boldsymbol{\sigma}_t, \boldsymbol{\tau}_t$ stand respectively for twice the spin and isospin operators of particle t .

With the techniques described before we are able to evaluate the matrix elements of the Hamiltonian given in Eq. (14.7). To deal with the 1st term just remember that

$$\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = \frac{1}{2} [4S^2 - (\boldsymbol{\sigma}_1)^2 - (\boldsymbol{\sigma}_2)^2] = 2S(S+1) - 3, \quad (14.8)$$

and similarly,

$$\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = 2T(T+1) - 3. \quad (14.9)$$

The results obtained by Elliott and Flowers in ref. [10] are shown in Fig. II.3. They used for the frequency the value $(\hbar/m\omega)^{1/2} = 1.64$ fm. The curves characterized by J and T were obtained by carrying out the calculations for different values V_0 of the residual interaction. We note incidentally that the evaluation of the relevant matrix elements requires the Talmi integrals for a Yukawa potential which are given in (2.10). The energy levels graphed were obtained for $V_0 = 42$ MeV and are compared with experiment. It should be noted that the techniques we have developed above were not available to Elliott and Flowers. They had to resort to the laborious evaluation of the radial matrix elements in terms of Laguerre polynomials plus the standard Racah analysis for the angular part.

15 Transformation Brackets for Arbitrary Angles in Terms of Standard Transformation Brackets

In section 10 we discussed the transformation brackets from two-particle states in terms of coordinates $\mathbf{x}_1, \mathbf{x}_2$ to those in terms of $\dot{\mathbf{x}}_1, \dot{\mathbf{x}}_2$ related to the first by

$$\begin{pmatrix} \dot{\mathbf{x}}_1 \\ \dot{\mathbf{x}}_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}. \quad (15.1)$$

This equation shows that in the two-dimensional space of the particle indices we have made a rotation by $\pi/4$.

In this section we shall derive the transformation brackets when the relation between coordinates is given by the general orthogonal matrix

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2}\beta & -\sin \frac{1}{2}\beta \\ \sin \frac{1}{2}\beta & \cos \frac{1}{2}\beta \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad (15.2)$$

where the angle of rotation is now $\beta/2$.

We shall present an analysis, discussed by A. Gal [11], in which the transformation brackets associated with (15.2) are given in terms of the transformation brackets associated with (15.1); in this section, we refer to the latter as standard transformation brackets (STB).

From the analysis of section 10 we recall that the two-particle states can be written as

$$|n_1 l_1, n_2 l_2, \Lambda M\rangle = P(n_1 l_1, n_2 l_2, \Lambda M)|0\rangle, \quad (15.3)$$

where P is the polynomial

$$\begin{aligned} P(n_1 l_1, n_2 l_2, \Lambda M) = \\ A_{n_1 l_1} A_{n_2 l_2} (\eta_1 \cdot \eta_1)^{n_1} (\eta_2 \cdot \eta_2)^{n_2} [\mathcal{Y}_{l_1}(\eta_1) \mathcal{Y}_{l_2}(\eta_2)]_{\Lambda M}. \end{aligned} \quad (15.4)$$

From the definition (8.8) of η in terms of x and p , it is clear that the transformation (15.2) for the coordinates induces a similar one for the creation operators, i.e.,

$$\begin{pmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix} = \begin{pmatrix} \cos \frac{1}{2}\beta & -\sin \frac{1}{2}\beta \\ \sin \frac{1}{2}\beta & \cos \frac{1}{2}\beta \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}. \quad (15.5)$$

The transformation bracket for rotations by an angle $\beta/2$ will be designated by

$$\langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle_\beta, \quad (15.6)$$

and it clearly connects the polynomials

$$\begin{aligned} P(n_1 l_1, n_2 l_2, \Lambda M) = \\ \sum_{\substack{n'_1 l'_2 \\ l'_1 l'_2}} \dot{P}(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M) \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle_\beta, \end{aligned} \quad (15.7)$$

where \dot{P} is defined by (15.4) with η_s replacing $\eta_s, s = 1, 2$ and we expand η_s in terms of $\dot{\eta}_s$ rather than the other way around.

To find the brackets (15.6) in terms of STB, we decompose the reciprocal of (15.5):

$$\begin{aligned} \begin{pmatrix} \cos \frac{1}{2}\beta & \sin \frac{1}{2}\beta \\ -\sin \frac{1}{2}\beta & \cos \frac{1}{2}\beta \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & -i \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix} \\ &\times \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} e^{-\frac{1}{2}i\beta} & 0 \\ 0 & e^{\frac{1}{2}i\beta} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \\ &= ABCDEFG, \end{aligned} \quad (15.8)$$

where the capital letters in (15.8) correspond to the matrices in the order indicated. We see at once that the matrices C, F lead to STB. The effect of matrices A, G is just to multiply the polynomial P by $(\mp i)^{2n_2+l_2}$, respectively, as the degree of the polynomial in η_2 is $2n_2+l_2$. For a similar reason the effect of E is to multiply the polynomial by the phase factor

$$(e^{\frac{1}{2}i\beta})^{2n_2+l_2-2n_1-l_1}. \quad (15.9)$$

Finally the effect of $D = B$ is to exchange η_1, η_2 . Equation (15.4) then shows that

$$DP(n_1 l_1, n_2 l_2, \Lambda M) = (-1)^{l_1+l_2-\Lambda} P(n_2 l_2, n_1 l_1, \Lambda M). \quad (15.10)$$

Combining all of these results and using the following symmetry relations of the STB (derived from (10.38)),

$$\begin{aligned} \langle \dot{n}_2 \dot{l}_2, \dot{n}_1 \dot{l}_1, \Lambda | n_2 l_2, n_1 l_1, \Lambda \rangle &= (-1)^{l_2+i_2} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle \\ \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle &= (-1)^{l_2+i_2} \langle n_1 l_1, n_2 l_2, \Lambda | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda \rangle \\ \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle &= (-1)^{l_1-\Lambda} \langle \dot{n}_2 \dot{l}_2, \dot{n}_1 \dot{l}_1, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle \end{aligned} \quad \left. \right\}, \quad (15.11)$$

we obtain finally

$$\begin{aligned} &\langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle_\beta \\ &= i^{2\dot{n}_1+\dot{l}_2-2n_2-l_2} \sum_{\substack{n'_1 l'_2 \\ n'_2 l'_1}} \exp[\frac{1}{2}i\beta(2n'_2 + l'_2 - 2n'_1 - l'_1)](-1)^{l_2+i_2} \\ &\times \langle n'_1 l'_1, n'_2 l'_2, \Lambda | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda \rangle \langle n'_1 l'_1, n'_2 l'_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle. \end{aligned} \quad (15.12)$$

The last equation of (15.11) may be used to show that this transformation bracket only takes real values. If a term $n'_1 l'_1 n'_2 l'_2$ occurs in the summation in (15.12), then $n'_2 l'_2 n'_1 l'_1$ will occur also; but using the last equation of (15.11) twice, these two terms will have the same sign if $l_1 + l'_1$ is even, so that only the cosine term of the exponential survives; while if $l_1 + l'_1$ is odd, i times the sine term survives. However, energy conservation implies

$$2n_1 + l_1 + 2n_2 + l_2 = 2n_1 + l_1 + 2n_2 + l_2 = 2n'_1 + l'_1 + 2n'_2 + l'_2, \quad (15.13)$$

and thus

$$(-1)^{l_1+l_1} = (-1)^{l_2+l_2}. \quad (15.14)$$

Hence the power of i outside the sum in (15.12) is real for cosine terms in the sum, imaginary for sine terms, and the resultant transformation bracket is always real.

There are many applications of these transformation bracket [11,12], but we shall give particular stress to a new one when discussing the three- and four-body problems.

Note that in this discussion we have used angles of $\beta/2$, in order to conform to the notation used by Gal [11].

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Chapter III

The Three-Body Problem

In this chapter we derive complete sets of three particle harmonic oscillator states in configuration space that have definite total orbital angular momentum and are bases for irreducible representations of the group $S(3)$ of permutations of three objects. We then proceed to apply these states in a number of problems of physical interest.

As a first step we consider translationally invariant problems where we eliminate the centre-of-mass variable, thus having a system with one coordinate less. Much of the discussion of the following sections is done for systems of n particles and then particularized to the cases of three and four particles in this and the next chapters.

16 Matrix Elements of the Hamiltonian with Respect to Translationally Invariant States

In this section we will outline a general procedure for getting the matrix elements of the intrinsic Hamiltonian of an n -particle problem with respect to translationally invariant harmonic oscillator states. For this purpose we consider first the Hamiltonian \mathcal{H} of an auxiliary problem of n particles of mass m interacting through harmonic oscillator forces of frequency ω/\sqrt{n} :

$$\mathcal{H} = \sum_{s=1}^n \frac{1}{2m} (\mathbf{p}'_s)^2 + \frac{m\omega^2}{2n} \sum_{s < t}^n (\mathbf{x}'_s - \mathbf{x}'_t)^2, \quad (16.1)$$

where \mathbf{x}', \mathbf{p}' are in ordinary units while \mathbf{x}, \mathbf{p} are dimensionless, as in section 3. Introducing the Jacobi coordinates [1]

$$\left. \begin{aligned} \dot{\mathbf{x}}_s &\equiv [s(s+1)]^{-\frac{1}{2}} \left[\sum_{t=1}^s \mathbf{x}_t - s\mathbf{x}_{s+1} \right], \quad 1 \leq s \leq n-1 \\ \dot{\mathbf{x}}_n &\equiv \frac{1}{\sqrt{n}} \sum_{t=1}^n \mathbf{x}_t, \end{aligned} \right\} \quad (16.2)$$

and similar definitions for the Jacobi momenta \mathbf{p}_s , the Hamiltonian \mathcal{H} becomes

$$\mathcal{H} = \frac{1}{2}\hbar\omega \sum_{s=1}^{n-1} [(\dot{\mathbf{p}}_s)^2 + (\dot{\mathbf{x}}_s)^2] + \frac{1}{2}\hbar\omega(\dot{\mathbf{p}}_n)^2. \quad (16.3)$$

The last term in (16.3) is the kinetic energy of the centre-of-mass motion:

$$\frac{1}{2}\hbar\omega(\dot{\mathbf{p}}_n)^2 = \frac{1}{2nm} \left[\sum_{s=1}^n \mathbf{p}'_s \right]^2. \quad (16.4)$$

If we want to deal only with intrinsic eigenstates of \mathcal{H} , *i.e.*, those that are translationally invariant, they will be given by the product of single-coordinate states

$$\prod_{s=1}^{n-1} \langle \dot{\mathbf{x}}_s | \dot{n}_s \dot{l}_s m_s \rangle. \quad (16.5)$$

Linear combinations of products of the states (16.5) with the corresponding spin and, if necessary, isospin parts, provide a complete set of translationally invariant states. We shall further characterize these states by means of the total number of quanta

$$\mathfrak{N} = \sum_{s=1}^{n-1} (2\dot{n}_s + \dot{l}_s), \quad (16.6)$$

the total angular momentum J and its projection M , and by antisymmetry under exchange of coordinates, spins and isospins, in order to satisfy the Pauli principle. We shall use the symbol \mathcal{N} to designate generically *all* the quantum numbers in these translationally invariant n -particle states, so that they can be represented by the ket

$$|\mathcal{N}\rangle = |\mathfrak{N}JM\dots\rangle, \quad (16.7)$$

with the dots standing for all the other quantum numbers that characterize the state. We shall later on indicate how to get states of the type (16.7) in an explicit fashion for three- and four-particle systems.

We turn now to a realistic n -particle translationally invariant Hamiltonian:

$$H = \frac{1}{2m} \sum_{s=1}^n (\mathbf{p}'_s)^2 + \sum_{s < t=2}^n V(s, t), \quad (16.8)$$

where $V(s, t)$ can depend on the relative coordinates and momenta, *i.e.*, $\mathbf{x}'_s - \mathbf{x}'_t$, $\mathbf{p}'_s - \mathbf{p}'_t$ of particles s, t as well as on their spins and isospins as discussed, for example, in section 14.

We are usually only interested in the intrinsic part H_I of the Hamiltonian H , which is obtained when we subtract from H the centre-of-mass kinetic energy (16.4). Furthermore, to simplify the following analysis, let us add and subtract from H_I the potential term in (16.1), thus getting from (16.3)

$$H_I \equiv H - \frac{1}{2nm} \left(\sum_{s=1}^n \mathbf{p}'_s \right)^2 = \frac{1}{2}\hbar\omega \sum_{s=1}^{n-1} [(\dot{\mathbf{p}}_s)^2 + (\dot{\mathbf{x}}_s)^2] + \sum_{s < t=2}^n U(s, t), \quad (16.9)$$

with

$$U(s, t) \equiv V(s, t) - \frac{m\omega^2}{2n} (\mathbf{x}'_s - \mathbf{x}'_t)^2. \quad (16.10)$$

We now proceed to calculate the matrix elements of H_I with respect to $|\mathcal{N}\rangle$; remembering that this state is completely antisymmetric under interchange of coordinates, spins and isospins, we get

$$\langle \mathcal{N}' | H_I | \mathcal{N} \rangle = \hbar\omega [\mathfrak{N} + \frac{3}{2}(n-1)] \delta_{\mathcal{N}', \mathcal{N}} + \frac{1}{2}n(n-1) \langle \mathcal{N}' | U(1, 2) | \mathcal{N} \rangle. \quad (16.11)$$

Here $\delta_{\mathcal{N}', \mathcal{N}}$ is a symbol that denotes the products of Kronecker deltas of all the quantum numbers in (16.7), while $\frac{1}{2}n(n-1)$ is the number of pairs, and

$$U(1, 2) = V(\dot{\mathbf{x}}_1, \dot{\mathbf{p}}_1, \mathbf{s}_1 + \mathbf{s}_2, \mathbf{t}_1 + \mathbf{t}_2) - n^{-1}\hbar\omega(\dot{\mathbf{x}}_1)^2. \quad (16.12)$$

In (16.12) $\mathbf{s}_1, \mathbf{s}_2$ and $\mathbf{t}_1, \mathbf{t}_2$ are the spins and isospins of the two particles, and, from (16.2),

$$\dot{\mathbf{x}}_1 = \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2), \quad \dot{\mathbf{p}}_1 = \frac{1}{\sqrt{2}}(\mathbf{p}_1 - \mathbf{p}_2). \quad (16.13)$$

Clearly therefore the matrix element of $U(1, 2)$ in (16.11) can be reduced to one-body matrix elements of the type discussed in section 14.

Applications of (16.11) to calculation of energy levels of four-particle systems have been given elsewhere [2]. Other applications related to the binding energy of the α particle and the possible determination of its ground state will be mentioned at the end of chapter IV.

17 Translationally Invariant Three-Particle States of Definite Permutational Symmetry

Particularizing the analysis of the previous section to three particles, the configuration part of the translationally invariant states can be expanded in terms of the states

$$\langle \dot{\mathbf{x}}_1 | \dot{n}_1 \dot{l}_1 \dot{m}_1 \rangle \langle \dot{\mathbf{x}}_2 | \dot{n}_2 \dot{l}_2 \dot{m}_2 \rangle, \quad (17.1)$$

or alternatively in terms of states coupled to a total orbital angular momentum Λ and projection M , i.e.,

$$|\dot{n}_1 \dot{l}_1 \dot{n}_2 \dot{l}_2, \Lambda M\rangle \equiv [\langle \dot{\mathbf{x}}_1 | \dot{n}_1 \dot{l}_1 \rangle \langle \dot{\mathbf{x}}_2 | \dot{n}_2 \dot{l}_2 \rangle]_{\Lambda M}, \quad (17.2)$$

where, from (16.2),

$$\dot{\mathbf{x}}_1 = \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2), \quad \dot{\mathbf{x}}_2 = \frac{1}{\sqrt{6}}(\mathbf{x}_1 + \mathbf{x}_2 - 2\mathbf{x}_3). \quad (17.3)$$

The ket (17.2) can also be expressed, as indicated in sections 10 or 15, as a polynomial \dot{P} in the creation operators

$$\dot{\eta}_s = \frac{1}{\sqrt{2}}(\dot{\mathbf{x}}_s - i\dot{\mathbf{p}}_s), \quad s = 1, 2, \quad (17.4)$$

acting on the ground state $|0\rangle$:

$$|\dot{n}_1 \dot{l}_1 \dot{n}_2 \dot{l}_2, \Lambda M\rangle = \dot{P}(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M)|0\rangle, \quad (17.5)$$

where, as in (15.4), \dot{P} is given by

$$\begin{aligned} \dot{P}(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M) \\ = A_{\dot{n}_1 \dot{l}_1} A_{\dot{n}_2 \dot{l}_2} (\dot{\eta}_1 \cdot \dot{\eta}_1)^{\dot{n}_1} (\dot{\eta}_2 \cdot \dot{\eta}_2)^{\dot{n}_2} [\mathcal{Y}_{l_1}(\dot{\eta}_1) \mathcal{Y}_{l_2}(\dot{\eta}_2)]_{\Lambda M}, \end{aligned} \quad (17.6)$$

and

$$\begin{aligned} |0\rangle &= \pi^{-\frac{3}{2}} \exp\left\{-\frac{1}{2}[(\dot{\mathbf{x}}_1)^2 + (\dot{\mathbf{x}}_2)^2]\right\} \\ &= \pi^{-\frac{3}{2}} \exp\left\{-\frac{1}{2}[(\mathbf{x}_1)^2 + (\mathbf{x}_2)^2 + (\mathbf{x}_3)^2] - \frac{1}{3}(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3)^2\right\}. \end{aligned} \quad (17.7)$$

The ground state $|0\rangle$ is clearly invariant under permutation of the coordinates $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$, so that the discussion of the symmetry properties of linear combinations of kets (17.2) reduces to the analysis of the symmetry properties of the same linear combinations of polynomials \dot{P} . For example, if we

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want to symmetrise the polynomial $\dot{P}(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M)$ we have to apply all the six permutations of the group $S(3)$ to \dot{P} and then add the resulting polynomials. The corresponding symmetric state is obtained by applying the final polynomial to $|0\rangle$.

All elements of $S(3)$ can be built up from the transposition (1,2) and the cyclic permutation (1,2,3). From (17.3) and (17.4), these have the following effect on the creation operators:

$$\begin{aligned} (1, 2) \begin{pmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix} &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix}, \\ (1, 2, 3) \begin{pmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix} &= \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{pmatrix}. \end{aligned} \quad (17.8)$$

The effect of any permutation of $S(3)$ on \dot{P} can be obtained once we have the effect of (1,2) and (1,2,3) on this polynomial. But from (17.8) and the discussion of section 15, it is clear that the application of (1,2) to \dot{P} just multiplies it by $(-1)^{2\dot{n}_1 + \dot{l}_1}$, while the application of (1,2,3) to \dot{P} gives a linear combination of $\dot{P}'s$ whose coefficients are transformation brackets associated with an angle β such that

$$\cos \frac{1}{2}\beta = -\frac{1}{2}, \quad \sin \frac{1}{2}\beta = \frac{1}{2}\sqrt{3} \quad \text{or} \quad \frac{1}{2}\beta = \frac{2}{3}\pi. \quad (17.9)$$

Using these results, we could build up in a straightforward but laborious manner the symmetrical state of the previous paragraph.

We shall show that a much simpler procedure for constructing the symmetrized state, or for that matter a three-particle translationally invariant harmonic oscillator state of arbitrary symmetry, can be obtained if we introduce the auxiliary operators

$$\left. \begin{aligned} \eta_1 &\equiv \frac{1}{\sqrt{2}}(-i\dot{\eta}_1 + \dot{\eta}_2) \\ \eta_2 &\equiv \frac{1}{\sqrt{2}}(i\dot{\eta}_1 + \dot{\eta}_2) \end{aligned} \right\}. \quad (17.10)$$

In this section η_1 and η_2 will be given by the definition (17.10) and are not to be confused with creation operators associated with the coordinates $\mathbf{x}_1, \mathbf{x}_2$. From (17.8) it is clear that under the generators of $S(3)$, η_1, η_2 transform as

$$\begin{aligned} (1, 2) \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}; \\ (1, 2, 3) \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} &= \begin{pmatrix} e^{-\frac{2}{3}\pi i} & 0 \\ 0 & e^{\frac{2}{3}\pi i} \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix}. \end{aligned} \quad (17.11)$$

We now consider polynomials $P(n_1 l_1, n_2 l_2, \Lambda M)$ that are defined in exactly the same way as (17.6), but with η_s, n_s, l_s replacing $\dot{\eta}_s, \dot{n}_s, \dot{l}_s, s = 1, 2$. The application of (1.2), (1.2,3) to P means carrying out the inverse operation [3] on η_1, η_2 ; so from (17.11) and the discussion in section 15 we get

$$(1, 2)P(n_1 l_1, n_2 l_2, \Lambda M) = (-1)^{l_1 + l_2 - \Lambda} P(n_2 l_2, n_1 l_1, \Lambda M), \quad (17.12)$$

$$(1, 2, 3)P(n_1 l_1, n_2 l_2, \Lambda M) = \exp(4\pi i g/3)P(n_1 l_1, n_2 l_2, \Lambda M), \quad (17.13)$$

where

$$2g \equiv 2n_1 + l_1 - 2n_2 - l_2. \quad (17.14)$$

To obtain polynomials of definite permutational symmetry we require appropriate projection operators. We refer the reader to Hamermesh's book [4], where the projection operator \mathcal{P}^f associated with a definite irreducible representation f of a finite group G is given. It is

$$\mathcal{P}^f \equiv \frac{d_f}{[G]} \sum_p \chi^{f*}(p)p, \quad (17.15)$$

where p is an element of the group, $\chi^f(p)$ the character associated with this element for the irreducible representation f , $[G]$ is the order of group and d_f the dimension of the irreducible representation f .

For the group of permutations $S(3)$ there are three irreducible representations [5] characterized by the partitions $f = \{3\}, \{21\}$ and $\{111\}$. Their dimensions d_f are 1, 2 and 1, respectively. The first and third are the familiar completely symmetric and antisymmetric representations. From the table of characters of $S(3)$ given, for example, in Hamermesh [5], we get for the projection operators of $S(3)$

$$\mathcal{P}^{\{3\}} = \frac{1}{6}[e + (1, 2) + (1, 3) + (2, 3) + (1, 2, 3) + (1, 3, 2)], \quad (17.16)$$

$$\begin{aligned} \mathcal{P}^{\{21\}} &= \frac{1}{3}[2e - (1, 2, 3) - (1, 3, 2)] \\ &= \frac{1}{3}[2e - (1, 2, 3) - (1, 2, 3)^{-1}], \end{aligned} \quad (17.17)$$

$$\mathcal{P}^{\{111\}} = \frac{1}{6}[e - (1, 2) - (1, 3) - (2, 3) + (1, 2, 3) + (1, 3, 2)], \quad (17.18)$$

where e is the identity element.

We shall first apply $\mathcal{P}^{\{21\}}$ to the polynomial $P(n_1 l_1, n_2 l_2, \Lambda M)$. From (17.13) we have

$$\begin{aligned} \mathcal{P}^{\{21\}}P(n_1 l_1, n_2 l_2, \Lambda M) &= \frac{1}{3}(2 - e^{\frac{4}{3}\pi i g} - e^{-\frac{4}{3}\pi i g})P(n_1 l_1, n_2 l_2, \Lambda M) \\ &= \frac{4}{3}\sin^2(\frac{2}{3}\pi g)P(n_1 l_1, n_2 l_2, \Lambda M) \\ &= (1 - \delta_{\nu 0})P(n_1 l_1, n_2 l_2, \Lambda M), \end{aligned} \quad (17.19)$$

where ν is defined by the congruence relation

$$2g \equiv \nu \pmod{3}. \quad (17.20)$$

From (17.19) we see that ν must be either 1 or 2, for when $\nu = 0$ the projected state of partition $\{21\}$ vanishes.

As the dimensionality of the irreducible representation $f = \{21\}$ of $S(3)$ is $d_f = 2$, we have two states in it that are characterized by the Young tableaux [6]

$$\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array} \longleftrightarrow (211); \quad \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \hline \end{array} \longleftrightarrow (121). \quad (17.21)$$

They could also be characterized by the Yamanouchi symbols $(r_3 r_2 r_1)$ which specify the row in which we find each of the numbers 3,2,1; these symbols are also indicated in (17.21).

From the Young tableaux one concludes that the states characterized by the Yamanouchi symbols (211) and (121) are respectively symmetric and antisymmetric under exchange of particles 1 and 2. To get then the states characterized by (211) and (121), we need to apply to the polynomials $P(n_1 l_1, n_2 l_2, \Lambda M)$ with $\nu = 1, 2$ the projection operators that give states symmetric or antisymmetric in the first two particles:

$$\mathcal{P}^{\{2\}} = \frac{1}{2}[e + (1, 2)], \quad \mathcal{P}^{\{11\}} = \frac{1}{2}[e - (1, 2)]. \quad (17.22)$$

From (17.12) this immediately gives for $\nu \neq 0$

$$\begin{aligned} \mathcal{P}^{\{2\}}P(n_1 l_1, n_2 l_2, \Lambda M) &= \frac{1}{2}[P(n_1 l_1, n_2 l_2, \Lambda M) + (-1)^{l_1 + l_2 - \Lambda} P(n_2 l_2, n_1 l_1, \Lambda M)] \\ &\equiv \frac{1}{\sqrt{2}}\phi(n_1 l_1, n_2 l_2, \Lambda M; \{21\}(211)), \end{aligned} \quad (17.23)$$

$$\begin{aligned} \mathcal{P}^{\{11\}}P(n_1 l_1, n_2 l_2, \Lambda M) &= \frac{1}{2}[P(n_1 l_1, n_2 l_2, \Lambda M) - (-1)^{l_1 + l_2 - \Lambda} P(n_2 l_2, n_1 l_1, \Lambda M)] \\ &\equiv \frac{i}{\sqrt{2}}(-1)^\nu \phi(n_1 l_1, n_2 l_2, \Lambda M; \{21\}(121)). \end{aligned} \quad (17.24)$$

In (17.23) and (17.24), the ϕ are the normalized polynomials characterized by the partition $\{21\}$ and the corresponding Yamanouchi symbol, as well as by $n_1 l_1, n_2 l_2, \Lambda M$; recall here that $P(n_1 l_1, n_2 l_2, \Lambda M)$ is never equal to $P(n_2 l_2, n_1 l_1, \Lambda M)$ since $\nu \equiv 2n_1 + l_1 - 2n_2 - l_2 \neq 0$. In (17.24) the phase factor is prescribed by the ladder procedure [1].

To get the symmetric and antisymmetric states we could apply $\mathcal{P}^{\{3\}}$ and $\mathcal{P}^{\{111\}}$ respectively, remembering that all permutations can be expressed in

terms of (1,2) and (1,2,3). However, a more elegant procedure is to note that from the analysis carried out for $f = \{21\}$ we conclude that only linear combinations of polynomials $P(n_1 l_1, n_2 l_2, \Lambda M)$ for which $2n_1 + l_1 - 2n_2 - l_2 \equiv 0 \pmod{3}$ would be either symmetric or antisymmetric. Those that are symmetric are characterized by the Young tableau

$$\begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline \end{array} \longleftrightarrow (111), \quad (17.25)$$

and thus are also symmetric under permutation of particles 1 and 2, as is quite obvious. Those that are antisymmetric are characterized by the Young tableau

$$\begin{array}{|c|} \hline 1 \\ \hline 2 \\ \hline 3 \\ \hline \end{array} \longleftrightarrow (321), \quad (17.26)$$

and are antisymmetric under permutation of particles 1 and 2, as is also obvious. We can then get the $\{3\}(111)$ and $\{111\}(321)$ normalized states by applying respectively the operators $\mathcal{P}^{\{2\}}$ and $\mathcal{P}^{\{11\}}$ of (17.22) to the polynomial $P(n_1 l_1, n_2 l_2, \Lambda M)$, i.e.,

$$\begin{aligned} & \left[\begin{array}{c} \mathcal{P}^{\{2\}} \\ \mathcal{P}^{\{11\}} \end{array} \right] P(n_1 l_1, n_2 l_2, \Lambda M) \\ &= \frac{1}{2} [P(n_1 l_1, n_2 l_2, \Lambda M) \pm (-1)^{l_1+l_2-\Lambda} P(n_2 l_2, n_1 l_1, \Lambda M)] \\ &= \frac{1}{\sqrt{2}} \left[\begin{array}{c} \phi(n_1 l_1, n_2 l_2, \Lambda M; \{3\}(111)) \\ \phi(n_1 l_1, n_2 l_2, \Lambda M; \{111\}(321)) \end{array} \right]. \end{aligned} \quad (17.27)$$

The expression (17.27) is valid when $2n_1 + l_1 - 2n_2 - l_2 \equiv 0 \pmod{3}$ but with the pair $(n_1 l_1)$ different from $(n_2 l_2)$. When

$$n_1 = n_2 = n, \quad l_1 = l_2 = l, \quad (17.28)$$

we get from (17.27)

$$P(nl, nl, \Lambda M) = \begin{cases} \phi(nl, nl, \Lambda M; \{3\}(111)) & \text{if } \Lambda \text{ even,} \\ \phi(nl, nl, \Lambda M; \{111\}(321)) & \text{if } \Lambda \text{ odd.} \end{cases} \quad (17.29)$$

Thus we have obtained polynomials with definite permutational symmetry for the three-particle translationally invariant problem in terms of the creation operators η_1, η_2 of (17.10). For the calculation of the matrix elements of the Hamiltonian (16.11), as well as for the nuclear form factor to be discussed in section 19, it is much more convenient to have the polynomials expressed in terms of the creation operators $\dot{\eta}_1, \dot{\eta}_2$, that is, in terms of

$\dot{P}(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M)$. This is easily achieved when we realize that the transformation matrix (17.10) connecting η_1, η_2 with $\dot{\eta}_1, \dot{\eta}_2$ can be decomposed in the following form:

$$\begin{pmatrix} -i/\sqrt{2} & \sqrt{\frac{1}{2}} \\ i/\sqrt{2} & \sqrt{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} -i & 0 \\ 0 & 1 \end{pmatrix} \equiv AB. \quad (17.30)$$

This problem is much simpler than that discussed in section 15. The application of A to P gives a linear combination of P 's whose coefficients are standard transformation brackets (STB), while the effect of B is just to multiply the polynomial by $(-i)^{2\dot{n}_1 + \dot{l}_1}$. Combining these two operations, we arrive at the result

$$\begin{aligned} P(n_1 l_1, n_2 l_2, \Lambda M) &= \sum_{\substack{\dot{n}_1 \dot{l}_1 \\ \dot{n}_2 \dot{l}_2}} P(\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M) \\ &\times (-1)^{\dot{n}_1 + \dot{l}_1} i^{\dot{l}_1} \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle, \end{aligned} \quad (17.31)$$

where we also made use of the symmetry relation (15.11) of the STB.

From (17.31) and this discussion we see that

$$\begin{aligned} |n_1 l_1, n_2 l_2, \Lambda M; fr\rangle &\equiv \phi(n_1 l_1, n_2 l_2, \Lambda M; f, r)|0\rangle \\ &= A(\nu, f, r)[P(n_1 l_1, n_2 l_2, \Lambda M) \pm (-1)^{l_1+l_2-\Lambda} P(n_2 l_2, n_1 l_1, \Lambda M)]|0\rangle \\ &= \sum_{\substack{\dot{n}_1 \dot{n}_2 \\ \dot{l}_1 \dot{l}_2}} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M\rangle \\ &\times \{A(\nu, f, r)(-1)^{\dot{n}_1 + \dot{l}_1} i^{\dot{l}_1} [1 \pm (-1)^{\dot{l}_1}] \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda \rangle\} \\ &\equiv \sum_{\substack{\dot{n}_1 \dot{n}_2 \\ \dot{l}_1 \dot{l}_2}} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M\rangle \\ &\times \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda, f, r \rangle, \end{aligned} \quad (17.32)$$

where f and r are shorthand notations for the partitions $\{f_1 f_2 f_3\}$ and Yamamoto symbols $(r_3 r_2 r_1)$; in deriving (17.32) we made use of a symmetry property of the transformation brackets [7]. The coefficient $A(\nu, f, r)$ and the value + or - in (17.32) are specified in (17.23, 24, 27). It is clear, incidentally, that the last transformation bracket in (17.32) is either real or pure imaginary, because the factor $[1 \pm (-1)^{\dot{l}_1}]$ restricts \dot{l}_1 to either even or odd values. We could then give a trivial redefinition of the ket (17.32), so that this transformation bracket is always real.

Let us designate by

$$|SM_S TM_T; fr\rangle \quad (17.33)$$

the three-particle spin-isospin state [8], with $SM_S(TM_T)$ being the total (isospin) and its projection and f, r having the same meaning as in the previous paragraph. The state completely antisymmetric under exchange of coordinates, spin and isospin [8] is then given by

$$|\mathcal{N}\rangle \equiv \frac{1}{\sqrt{d_f}} \sum_r (-1)^r |[n_1 l_1, n_2 l_2, \Lambda; fr] STM_T; \tilde{f} \tilde{r}]_{JM}\rangle. \quad (17.34)$$

In (17.34) \tilde{f}, \tilde{r} refer to the partition and Yamanouchi symbol associated with f and r ; if for instance $f, r = \{3\}, (111)$, then we have $\tilde{f}, \tilde{r} = \{111\}, (321)$. The phase $(-1)^r$ is defined in such way that $(-1)^r = +1, +1, +1, -1$ for $r = (111), (321), (211), (121)$, respectively. The symbol \mathcal{N} stands then for the set of quantum numbers

$$\mathcal{N} \equiv n_1 l_1 n_2 l_2 \Lambda f, STM_T, JM. \quad (17.35)$$

We have thus constructed explicitly the translationally invariant three-particle state of the general type discussed in section 16.

18 The General Three-Body Problem. Applications to the Lithium Atom

When dealing with nuclei we have a translationally invariant problem, as besides the kinetic energy we have only the interaction between nucleons. For this type of problem we can therefore use the translationally invariant states of sections 16 and 17.

In the atomic or molecular problem we have a fixed reference frame given by the coordinate system in which the nuclei of the atoms or molecules are fixed. If we then use the Jacobi coordinates (16.2) to describe the n -electron states, we must also include the centre-of-mass coordinate $\dot{\mathbf{x}}_n$. This coordinate is invariant under permutation of the original coordinates $\mathbf{x}_s, s = 1, 2, \dots, n$. Therefore the simplest way of constructing a state of definite symmetry and orbital angular momentum in configuration space is to have a state of this type for the $n-1$ translationally invariant coordinates $\dot{\mathbf{x}}_s, s = 1, 2, \dots, n-1$, and couple its angular momentum with the l of the single-coordinate state in $\dot{\mathbf{x}}_n$.

For the three-particle problem the translationally invariant states are given by the ket of (17.32), so the procedure of the previous paragraph leads to the state

$$|n_1 l_1, n_2 l_2(\Lambda); n_3 l_3; \ell m; fr\rangle = [\langle \dot{\mathbf{x}}_1 \dot{\mathbf{x}}_2 | n_1 l_1, n_2 l_2, \Lambda; fr \rangle \langle \dot{\mathbf{x}}_3 | n_3 l_3 \rangle]_{\ell m}, \quad (18.1)$$

where the square bracket stands for the vector coupling of Λ and l_3 to a total orbital angular momentum ℓ and projection m and the first bracket is given by (17.32).

The state $\phi|0\rangle$ of (17.32) can be decomposed in terms of the states

$$|\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M\rangle$$

of (17.2) with the help of the brackets

$$\langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda | n_1 l_1, n_2 l_2, \Lambda; fr \rangle \quad (18.2)$$

defined in (17.32).

From the definition (18.1) of the general three-particle state we see that we can use the same bracket (18.2) to decompose the ket (18.1) in terms of the state

$$\begin{aligned} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2(\Lambda); n_3 l_3; \ell m\rangle &= [[\langle \dot{\mathbf{x}}_1 | \dot{n}_1 \dot{l}_1 \rangle \langle \dot{\mathbf{x}}_2 | \dot{n}_2 \dot{l}_2 \rangle]_\Lambda \langle \dot{\mathbf{x}}_3 | n_3 l_3 \rangle]_{\ell m} \\ &= \sum_{\bar{\Lambda}} [\langle \dot{\mathbf{x}}_1 | \dot{n}_1 \dot{l}_1 \rangle [\langle \dot{\mathbf{x}}_2 | \dot{n}_2 \dot{l}_2 \rangle \langle \dot{\mathbf{x}}_3 | n_3 l_3 \rangle]_{\bar{\Lambda}}]_{\ell m} \langle \dot{l}_1, \dot{l}_2 l_3(\bar{\Lambda}), \ell | \dot{l}_1 \dot{l}_2(\Lambda), l_3, \ell \rangle \\ &= \sum_{\bar{\Lambda}} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, n_3 l_3(\bar{\Lambda}); \ell m\rangle [(2\Lambda + 1) \\ &\quad \times (2\bar{\Lambda} + 1)]^{\frac{1}{2}} (-1)^{\dot{l}_1 + \dot{l}_2 + \ell + l_3} \left\{ \begin{array}{ccc} \dot{l}_1 & \dot{l}_2 & \Lambda \\ l_3 & \ell & \bar{\Lambda} \end{array} \right\}, \end{aligned} \quad (18.3)$$

where in the last lines we recoupled in the standard way [9] the single coordinate states with the help of the $6j$ coefficients $\left\{ \begin{array}{ccc} a & b & c \\ d & e & f \end{array} \right\}$.

We can now consider the matrix elements of a three-electron Hamiltonian in an atom or molecule with respect to the state (18.1). For the sake of definiteness let us consider the Hamiltonian of the lithium atom where (in the units of section 3) we have

$$H = \sum_{s=1}^3 \left[\frac{1}{2} \epsilon^2 (\mathbf{p}_s)^2 - \frac{\sqrt{2}\epsilon}{|\mathbf{x}_s|} \right] + \sum_{s < t=2}^3 \frac{\sqrt{2}\epsilon}{|\mathbf{x}_s - \mathbf{x}_t|}. \quad (18.4)$$

This Hamiltonian is invariant under rotation and permutation of the coordinates, so that ℓ, m, f in (18.1) will be good quantum numbers of H . The complete states of our three-electron problem are obtained when we multiply the configuration-space ket (18.1) by spin states equivalent to (17.33) and

then antisymmetrize, as in (17.34). When calculating the matrix elements of H , we can replace the first sum in (18.4) by three times the value of the square bracket for $s = 3$, because the states are antisymmetric under permutations of the particles and spins, and similarly the two-body interaction by three (the number of pairs) times the interaction between particles 1 and 2. Furthermore, since H is independent of the spin, the matrix elements reduce to those with respect to the states (18.1), but summed over the Yamanouchi symbol r . We thus get

$$\begin{aligned} & \sum_r \langle n'_1 l'_1, n'_2 l'_2(\Lambda'); n'_3 l'_3; \ell m; fr | H | n_1 l_1, n_2 l_2(\Lambda); n_3 l_3; \ell m; fr \rangle \\ &= 3 \sum_r \left\langle n'_1 l'_1, n'_2 l'_2(\Lambda'); n'_3 l'_3; \ell m; fr \left| \left[\frac{1}{2} \epsilon^2 (\mathbf{p}_3)^2 - \frac{\sqrt{2}\epsilon}{|\mathbf{x}_3|} \right] \right. \right. \\ & \quad \times n_1 l_1, n_2 l_2(\Lambda); n_3 l_3; \ell m; fr \left. \right\rangle \\ &+ 3 \sum_r \left\langle n'_1 l'_1, n'_2 l'_2(\Lambda'); n'_3 l'_3; \ell m; fr \left| \frac{\sqrt{2}\epsilon}{|\mathbf{x}_1 - \mathbf{x}_2|} \right. \right. \\ & \quad \times n_1 l_1, n_2 l_2(\Lambda); n_3 l_3; \ell m; fr \left. \right\rangle. \end{aligned} \quad (18.5)$$

Using the expansion of the states (18.1) in terms of the states (18.3) discussed above we see that the last term in (18.5) requires only the evaluation of the matrix element

$$\begin{aligned} & \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2(\Lambda'); n'_3 l'_3; \ell m | \frac{\epsilon}{|\mathbf{x}_1|} | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2(\Lambda); n_3 l_3; \ell m \rangle \\ &= \epsilon \sum_p B(\dot{n}'_1 \dot{l}'_1, \dot{n}_1 \dot{l}_1, p) \frac{p!}{\Gamma(p + \frac{3}{2})} \\ & \quad \times \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{n}'_2 \dot{n}_2} \delta_{\dot{l}'_2 \dot{l}_2} \delta_{n'_3 n_3} \delta_{l'_3 l_3} \delta_{\Lambda' \Lambda}. \end{aligned} \quad (18.6)$$

The first term on the right-hand side of (18.5) requires the recoupled states of the last line of (18.3), so we need only evaluate the matrix elements

$$\begin{aligned} & \langle \dot{n}'_1 \dot{l}'_1; \dot{n}'_2 \dot{l}'_2, n'_3 l'_3(\bar{\Lambda}'); \ell m | \frac{1}{2} \epsilon^2 (\mathbf{p}_3)^2 - \frac{\sqrt{2}\epsilon}{|\mathbf{x}_3|} | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, n_3 l_3(\bar{\Lambda}); \ell m \rangle \\ &= \langle \dot{n}'_2 \dot{l}'_2, n'_3 l'_3, \bar{\Lambda} \bar{M} | \frac{1}{2} \epsilon^2 (\mathbf{p}_3)^2 - \frac{\sqrt{2}\epsilon}{|\mathbf{x}_3|} | \right. \\ & \quad \times \dot{n}_2 \dot{l}_2, n_3 l_3, \bar{\Lambda} \bar{M} \rangle \delta_{\dot{n}'_1 \dot{n}_1} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\bar{\Lambda}' \bar{\Lambda}}. \end{aligned} \quad (18.7)$$

18. THE GENERAL THREE-BODY PROBLEM

Here the $\delta_{\bar{\Lambda}', \bar{\Lambda}}$ comes from the fact that the operator in the matrix element is a scalar.

To evaluate the last term in (18.7) we note that we can introduce the coordinates

$$\mathbf{X} \equiv \frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2), \quad \mathbf{x}_3, \quad (18.8)$$

related to $\dot{\mathbf{x}}_2, \dot{\mathbf{x}}_3$ by the transformation

$$\begin{pmatrix} \mathbf{X} \\ \mathbf{x}_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} \\ -\sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix} \begin{pmatrix} \dot{\mathbf{x}}_2 \\ \dot{\mathbf{x}}_3 \end{pmatrix}. \quad (18.9)$$

We then expand the states

$$\langle \dot{\mathbf{x}}_2 \dot{\mathbf{x}}_3 | \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3, \Lambda M \rangle \quad (18.10)$$

in terms of the states

$$\langle \mathbf{X} \mathbf{x}_3 | NL, nl, \Lambda M \rangle, \quad (18.11)$$

where the NL quantum numbers are associated with \mathbf{X} and nl with \mathbf{x}_3 . The expansion can be carried out with the help of the transformation brackets discussed in section 15:

$$\langle NL, nl, \Lambda | \dot{n}_2 \dot{l}_2, n_3 l_3, \Lambda \rangle_\beta, \quad (18.12)$$

where β is an angle such that

$$\cos \frac{1}{2}\beta = 1/\sqrt{3}, \quad \sin \frac{1}{2}\beta = -\sqrt{\frac{2}{3}}. \quad (18.13)$$

In this way the matrix element in (18.7) can be reduced to the matrix element

$$\left\langle n' l m | \frac{1}{2} \epsilon^2 p^2 - \frac{\sqrt{2}\epsilon}{r} | n l m \right\rangle \quad (18.14)$$

evaluated in section 3.

We have outlined a general procedure for evaluating the matrix elements (18.5), and we shall apply it to the evaluation of the energy of the ground state of the Li atom. This state has positive parity, total orbital angular momentum $l = 0$ and total spin $S = \frac{1}{2}$. The latter implies [10] that it must correspond to the partition $f = \{21\}$. As the parity of harmonic oscillators is connected with the number of quanta \mathfrak{N} — i.e., for positive (negative)

parity \mathfrak{N} is even (odd) — we are restricted to even \mathfrak{N} for the ground state of the Li atom. Now a state of $\mathfrak{N} = 0$ is proportional to

$$\exp[-\frac{1}{2}((x_1)^2 + (x_2)^2 + (x_3)^2)], \quad (18.15)$$

and thus symmetric under coordinate exchange, and so belongs to the partition $\{3\}$. Therefore it is excluded as a component of the Li ground state. The next possible value of \mathfrak{N} is 2, so the states (18.1) would be restricted by

$$2n_1 + l_1 + 2n_2 + l_2 + 2n_3 + l_3 = 2, \quad (18.16)$$

and, because of (17.19) and (17.20),

$$2n_1 + l_1 - 2n_2 - l_2 \not\equiv 0 \pmod{3}. \quad (18.17)$$

These conditions and the symmetrical form (17.23), (17.24) of the states belonging to $f = \{21\}$ leave us with the following states of the type (18.1):

$$\left| 10,00(0); 00; 00; \{21\}_r \right\rangle, \quad \left| 01,00(1); 01; 00; \{21\}_r \right\rangle, \quad (18.18)$$

with r having the values (211) and (121).

Restricting ourselves to $\mathfrak{N} = 2$, we obtain by the procedure discussed above a 2×2 matrix which is a function of ϵ . We can diagonalize it for selected values of ϵ , and minimizing it with respect to this parameter we get for the ground state energy of the Li atom a value [11] which is 60% of the experimental value. The calculation could be refined by going to larger values of \mathfrak{N} .

Applications to other three-electron atomic and molecular problems are given in reference [11].

19 Form Factors of Nuclei

In section 5 we discussed the scattering of electrons by hydrogen atoms and saw that from the ratio of the differential scattering cross section to the Rutherford cross section we could determine the form factor of the electron charge distribution. In a similar fashion [12] it is possible to show that the square root of the ratio of the differential scattering cross section of high-energy electrons by a nucleus to the corresponding Mott scattering by a point charge, determines up to a sign the value of the charge form factor of the nucleus defined by

$$F_{ch}(\mathbf{q}) \equiv \frac{1}{Z} \int \exp(i\mathbf{q} \cdot \mathbf{x}) \rho(\mathbf{x}) d\mathbf{x}. \quad (19.1)$$

Here Z is the number of protons in the nucleus, $\rho(\mathbf{x})$ the charge density referred to the centre of mass of the nucleus and $i\mathbf{q}$ is the momentum transfer (in units of $[\hbar m\omega]^{\frac{1}{2}}$, because \mathbf{x} is dimensionless).

In this section we shall indicate how we may obtain a theoretical expression for this form factor when we represent the ground state of the nucleus as a superposition of translationally invariant harmonic oscillator states of the type discussed in sections 16 and 17.

To carry out this programme, begin with the operators whose expectation values, with respect to the ground state of the nucleus, give us the probability density of finding either a proton or a neutron at a definite point in space $\tilde{\mathbf{x}}$. These operators are clearly

$$\hat{\Pi}_\nu(\tilde{\mathbf{x}}) = \sum_{s=1}^n \delta(\tilde{\mathbf{x}} - \mathbf{x}_s) [\frac{1}{2} + (-1)^\nu t_{0s}], \quad (19.2)$$

where \mathbf{x}_s, t_{0s} are respectively the position vector and the zero projection of isospin of particle s . In (19.2) the index ν takes the values $\nu = 0, 1$ with 0 and 1 characterizing respectively the neutron and proton operators. In other words, ν is the charge index. The number of nucleons is designated by n .

In the operator (19.2), the coordinate $\tilde{\mathbf{x}}$ is defined with respect to an arbitrary origin, while in the actual physical problem we are interested in the charge density referred to the centre of mass of the nucleus:

$$\mathbf{X} \equiv \frac{1}{n} \sum_{s=1}^n \mathbf{x}_s. \quad (19.3)$$

We shall therefore subtract \mathbf{X} from both $\tilde{\mathbf{x}}$ and \mathbf{x}_s in the δ function of (19.2). Defining now

$$\mathbf{x} \equiv \tilde{\mathbf{x}} - \mathbf{X} \quad (19.4)$$

as the coordinate with respect to the centre of mass of the nucleus, the operator (19.2) takes the form

$$\hat{\Pi}_\nu(\mathbf{x}) = \sum_{s=1}^n \delta[\mathbf{x} - (\mathbf{x}_s - \mathbf{X})] [\frac{1}{2} + (-1)^\nu t_{0s}]. \quad (19.5)$$

Our next step is to consider the expectation value of the operator $\hat{\Pi}_\nu(\mathbf{x})$ with respect to the ground state of the nucleus. This requires that we briefly discuss the latter. Among the good quantum numbers of the ground state are

the total angular momentum J and projection M , the parity π , the projection of the total isotopic spin

$$M_T = \frac{1}{2}(n - 2Z), \quad (19.6)$$

and, if we disregard Coulomb forces, the total isotopic spin T itself. The wave function with these quantum numbers may be expanded in terms of products of states in configuration and in spin-isospin space; it is clear that there are no spurious states if they are restricted to functions of only the relative coordinates, such as the Jacobi coordinates $\dot{\mathbf{x}}_s$, $s = 1, 2, \dots, n - 1$, of (16.2).

We characterize the configuration-space states by their permutational symmetry with respect to exchange of the coordinate, *i.e.*, by the partition f and Yamanouchi symbol r , as well as by the total orbital angular momentum L . The spin-isospin states will also be characterized by their permutational symmetry and total spin S and isospin T . According to the discussion leading to (17.34), the ground state will satisfy the Pauli principle if we expand it as

$$|\pi JMTM_T\rangle = \sum_{\alpha Lf} a(\alpha Lf\gamma S) \sum_{\gamma S} \frac{1}{\sqrt{d_f}} (-1)^r [|\alpha\pi Lfr\rangle |\gamma STM_T \tilde{f}\tilde{r}\rangle]_{JM}, \quad (19.7)$$

where α and γ indicate respectively all the other quantum numbers in the configuration and spin-isospin states and the a 's are the coefficients of the expansion restricted in the usual way by the normalization of the state (19.7). We suppress all fixed quantum number such as J, M , etc., in a . All other symbols have been discussed at the end of section 17, where they were particularized to the case $n = 3$. For the general case we only note that $(-1)^r$ is 1 or -1 , depending on whether we need an even or odd number of successive transpositions to take the Young tableau characterized by the Yamanouchi symbol r into the standard form in which the squares are numbered in succession 1, 2, 3, ..., in the first row, then the second, and so on [8]. As usual, the square bracket in (19.7) couples \mathbf{L} and \mathbf{S} to \mathbf{J} .

We are interested in the probability $\Pi_\nu(\mathbf{x})$ of observing a proton or a neutron in the nucleus, irrespective of the orientation of the nucleus in space. This means that we must take the expectation value of the operator $\hat{\Pi}_\nu(\mathbf{x})$ with respect to the states (19.7) and then average with respect to M ; we find that

$$\begin{aligned} \Pi_\nu(\mathbf{x}) &\equiv \frac{1}{2J+1} \sum_M \langle \pi JMTM_T | \hat{\Pi}_\nu(\mathbf{x}) | \pi JMTM_T \rangle \\ &= \frac{n}{2L+1} \sum_{\substack{f, f' \\ LS}} \sum_{\substack{\alpha, \alpha' \\ \gamma, \gamma'}} \sum_{\substack{rr' \\ \gamma\gamma'}} \sum_{M_L} \frac{(-1)^r (-1)^{r'}}{[d_f d_{f'}]^{\frac{1}{2}}} \\ &\times \left\langle \alpha' \pi LM_L f' r' | \delta \left(\mathbf{x} + \left[\frac{n-1}{n} \right]^{\frac{1}{2}} \dot{\mathbf{x}}_{n-1} \right) | \alpha \pi LM_L f r \right\rangle \\ &\times \langle \gamma' STM_T \tilde{f}' \tilde{r}' | (\frac{1}{2} + (-1)^\nu t_{0n}) | \gamma STM_T \tilde{f} \tilde{r} \rangle \\ &\times a^*(\alpha' Lf' \gamma' S) a(\alpha Lf \gamma S). \end{aligned} \quad (19.8)$$

The final form of $\Pi_\nu(\mathbf{x})$ in (19.8) is obtained from the following reasoning: As the states (19.7) are antisymmetric under exchange of coordinates, spin and isospin, we replace the operator (19.5) by n times the corresponding expression for $s = n$; from (16.2), this leads to the operator

$$n \delta \left(\mathbf{x} + \left[\frac{n-1}{n} \right]^{\frac{1}{2}} \dot{\mathbf{x}}_{n-1} \right) [\frac{1}{2} + (-1)^\nu t_{0n}] \quad (19.9)$$

appearing in (19.8). Furthermore, as (19.9) is independent of spin, the spin-isospin matrix element (19.8) is diagonal in S and independent of M_S . Thus from the vector coupling of \mathbf{L} , \mathbf{S} to \mathbf{J} in (19.7) we get in (19.8) a factor

$$\begin{aligned} &\frac{1}{2J+1} \sum_{MM_S} (-1)^{L-L'} (2J+1) \begin{pmatrix} L & S & J \\ M_L & M_S & -M \end{pmatrix} \begin{pmatrix} L' & S & J \\ M'_L & M_S & -M \end{pmatrix} \\ &= \frac{1}{2L+1} (-1)^{L-L'} \sum_{MM_S} (2L+1) \\ &\times \begin{pmatrix} S & J & L \\ M_S & -M & M_L \end{pmatrix} \begin{pmatrix} S & J & L' \\ M_S & -M & M'_L \end{pmatrix} \\ &= \delta_{LL'} \delta_{M_L M'_L} (2L+1)^{-1}. \end{aligned} \quad (19.10)$$

The actual charge density $\rho(\mathbf{x})$ in the nucleus is obtained from $\Pi_\nu(\mathbf{x})$, when we consider also the fact that protons or neutrons are not point particles but have a charge density of their own [13] which we indicate by $\rho_\nu(\mathbf{x})$ with $\nu = 1$ or 0. Thus we obtain

$$\rho(\mathbf{x}) = \int [\rho_1(\mathbf{x} - \mathbf{y}) \Pi_1(\mathbf{y}) + \rho_0(\mathbf{x} - \mathbf{y}) \Pi_0(\mathbf{y})] d\mathbf{y}. \quad (19.11)$$

Using the convolution theorem [14], the charge form factor can be written as

$$F_{ch}(\mathbf{q}) = f_1(\mathbf{q})F_1(\mathbf{q}) + f_0(\mathbf{q})F_0(\mathbf{q}), \quad (19.12)$$

where

$$f_\nu(\mathbf{q}) = \int \exp(i\mathbf{q} \cdot \mathbf{x})\rho_\nu(\mathbf{x})d\mathbf{x}, \quad (19.13)$$

$$F_\nu(\mathbf{q}) = \frac{1}{Z} \int \exp(i\mathbf{q} \cdot \mathbf{x})\Pi_\nu(\mathbf{x})d\mathbf{x}. \quad (19.14)$$

As $f_1(\mathbf{q})$, $f_0(\mathbf{q})$, which incidentally are only functions of \mathbf{q}^2 , have been obtained experimentally, we need only compute the theoretical $F_\nu(\mathbf{q})$, $\nu = 0, 1$, of (19.14), in order to compare the predictions to the experimental charge form factor. Introducing then (19.8) into (19.14) and interchanging the order of integration we see that $F_\nu(\mathbf{q})$ (which likewise is only a function of \mathbf{q}^2) can be written as

$$\begin{aligned} F_\nu(\mathbf{q}^2) &= \frac{1}{Z} \frac{n}{[d_f d_{f'}]^\frac{1}{2}} \sum_{ff'} \sum_{\alpha\alpha'} \sum_{LS} (-1)^r (-1)^{r'} \\ &\times \langle \alpha' \pi L f' r' | \frac{\sin \kappa |\dot{\mathbf{x}}_{n-1}|}{\kappa |\dot{\mathbf{x}}_{n-1}|} | \alpha \pi L f r \rangle \\ &\times \langle \gamma' S T M_T \tilde{f}' \tilde{r}' | \frac{1}{2} + (-1)^\nu t_{0n} | \gamma S T M_T \tilde{f} \tilde{r} \rangle \\ &\times a^*(\alpha' L f' \gamma' S) a(\alpha L f \gamma S). \end{aligned} \quad (19.15)$$

In (19.15) κ is given by

$$\kappa = q \sqrt{\frac{n-1}{n}} = q \left[\frac{\hbar(n-1)}{m\omega n} \right]^\frac{1}{2}, \quad (19.16)$$

where q is the momentum transfer in units of fm^{-1} . At first sight, instead of the operator appearing in the configuration-space matrix element in (19.15), we would have expected

$$\exp(i\kappa \cdot \dot{\mathbf{x}}_{n-1}) = \sum_{l=0}^{\infty} j_l(\kappa r) \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{lm}^*(\alpha, \beta) Y_{lm}(\theta, \varphi), \quad (19.17)$$

where (r, θ, φ) and (κ, α, β) are respectively the spherical coordinates associated with the vectors $\dot{\mathbf{x}}_{n-1}$ and κ ; $j_l(\kappa r)$ is the spherical Bessel function of order l . Let us evaluate separately the configuration-space matrix element for each term in the summation (19.17), getting from the Wigner-Eckart theorem [15] a factor $(-1)^{L-l+M_L} [2L+1]^\frac{1}{2} \times \begin{pmatrix} L & l & L \\ M_L & m & -M_L \end{pmatrix}$; this

19. FORM FACTORS OF NUCLEI

implies that only terms with $m = 0$ contribute. Furthermore, from (19.8) we see that we average over M_L , so that

$$\begin{aligned} &\frac{1}{2L+1} \sum_{M_L} (-1)^{L-l+M_L} [2L+1]^\frac{1}{2} \begin{pmatrix} L & l & L \\ M_L & 0 & -M_L \end{pmatrix} \\ &= \frac{1}{[2L+1]^\frac{1}{2}} \sum_{M_L} (-1)^{L+M_L} \begin{pmatrix} L & L & l \\ M_L & -M_L & 0 \end{pmatrix} \\ &= \sum_{M_L} \begin{pmatrix} L & L & 0 \\ M_L & -M_L & 0 \end{pmatrix} \begin{pmatrix} L & L & l \\ M_L & -M_L & 0 \end{pmatrix} = \delta_{l0}. \end{aligned} \quad (19.18)$$

We thus retain only the spherically symmetric term $j_0(\kappa r)$; hence the configuration-space matrix element in (19.15), which we now see is independent of M_L .

For the three-nucleon system $F_\nu(q^2)$ may be calculated immediately, using the explicit states (17.34). The configuration-space matrix elements reduce to

$$\langle n'lm | \frac{\sin \kappa r}{\kappa r} | nlm \rangle, \quad (19.19)$$

evaluated explicitly in (6.6–6.7), and the spin-isospin part can be calculated using the corresponding three-particle fractional-parentage coefficients [16].

Rather than discuss here applications of the general expression (19.15) for $F_\nu(q^2)$, we prefer to particularize it to the case where besides $\pi JMTM_T$ also L, S, f are good quantum numbers of our state and, besides, its configuration-space part is either symmetric or antisymmetric, i.e., $f = \{n\}$ or $\{1^n\}$. We have then $d_f = 1$ and we suppress the summations over the Yamanouchi symbols. Because $|\gamma S T M_T \tilde{f}\rangle$ will also be either symmetric or antisymmetric, we have

$$\begin{aligned} &n \langle \gamma' S T M_T \tilde{f} | \frac{1}{2} + (-1)^\nu t_{0n} | \gamma S T M_T \tilde{f} \rangle \\ &= \langle \gamma' S T M_T \tilde{f} | \sum_s (\frac{1}{2} + (-1)^\nu t_{0s}) | \gamma S T M_T \tilde{f} \rangle \\ &= [\frac{1}{2}n + (-1)^\nu M_T] \delta_{\gamma\gamma'} = \left\{ \frac{1}{2}[1 + (-1)^\nu]n - (-1)^\nu Z \right\} \delta_{\gamma\gamma'}. \end{aligned} \quad (19.20)$$

Thus we get in this particular case

$$F_\nu(q^2) = \sum_{\alpha\alpha'\gamma} \begin{bmatrix} (n-Z)/Z & \\ 1 & \end{bmatrix} \langle \alpha' \pi L f | \frac{\sin \kappa |\dot{\mathbf{x}}_{n-1}|}{\kappa |\dot{\mathbf{x}}_{n-1}|} | \alpha \pi L f \rangle a^*(\alpha' \gamma) a(\alpha \gamma), \quad (19.21)$$

where we have suppressed the fixed quantum numbers L, S, f in the coefficients a . For $\nu = 0$ ($\nu = 1$), *i.e.* the neutron (proton) distribution form factor, we take the upper (lower) term in the square bracket.

From (19.12) we see that if the proton and neutron are point particles with charges 1 and 0, we get for a state of fixed L, S and $f = \{n\}$ or $\{1^n\}$,

$$F_{ch}(q^2) = F_1(q^2), \quad (19.22)$$

with the latter given by (19.21). It is easily seen that this result continues to hold for any system of point particles of definite charge, such as for example the three-quark system of the proton, if the states in configuration space of the point particles are either symmetric or antisymmetric, so that we can use an argument similar to (19.20) for the internal coordinates of the point particles. We shall make use of this result when we discuss later the form factor of the proton in the quark model, while in the next section we discuss structure and form factor of 3H , 3He .

In the next chapter we shall also make use of (19.21) to discuss the form factor of the α particle, in whose ground state we shall assume $f = \{4\}$, $L = S = J = T = 0$.

20 Structure and Form Factor of 3H and 3He

a) Binding energy of 3H

In Section 17 the three-body harmonic oscillator wave functions were considered which are translationally invariant and allow us to calculate matrix elements of any Hamiltonian, as was discussed in Section 16.

Here we want to consider the applications of these wave functions and matrix elements to the calculation of the triton binding energy using a realistic nucleon-nucleon interaction. Such a calculation was done by Jackson, Lande and Sauer [17].

Jackson *et al.* [17] have used the Reid soft core potential [18] as a nucleon-nucleon interaction. This potential is chosen for each partial wave independently as a sum of Yukawa potentials. The asymptotic behavior of the potential in each partial wave corresponds to the one-pion exchange at large distances, while the short range components are fitted to experimental phase shifts. For example, the potential is of the following form for the 1S_0 channel:

$$V_{1S_0} = -10.463 \frac{e^{-\mu r}}{\mu r} - 1650.6 \frac{e^{-4\mu r}}{\mu r} + 6484.2 \frac{e^{-7\mu r}}{\mu r}, \quad (20.1)$$

where $\mu = 0.7 \text{ fm}^{-1}$.

Table III.1. Results of the variational calculations for triton properties. The terms $\langle V \rangle$ and $\langle r^2 \rangle^{1/2}$ give respectively the expectation values of the potential energy and the radius.

Binding energy B_T , MeV	6.30
Percentage of $\{21\}D$ States	8.9%
Percentage of $\{21\}S$ States	0.52%
$\langle V \rangle$ MeV	-56.11
$\langle r^2 \rangle^{1/2}$ fm	2.02

It is clear that any calculation of triton properties, which pretends to take into account the effects of short range two nucleon correlations with reasonable accuracy, should include states with a large number of oscillator quanta because the strength of the repulsive short range nuclear force, *i.e.*, the last term in (1), is rather high.

The oscillator frequency ω was considered as a variational parameter and the optimal value that was found for it in the case of the triton corresponds to a "radius" b of the value

$$b = \left(\frac{\hbar}{m\omega} \right)^{1/2} = 0.85 \text{ fm}, \quad (20.2)$$

where m is the mass of the proton.

A variational calculation of the binding energy was made with the help of matrix elements of the form (16.11).

Because of the large number of three-body harmonic oscillator states with a given maximal number of quanta a set of simplifications was done in [17].

Only states $\{3\}S$, $\{21\}D$ and $\{21\}S$ up to 34, 20 and 12 quanta respectively were included in the calculations. The Reid potential is not defined for partial waves with an orbital angular momentum $\ell \geq 3$. Therefore the contributions of all higher partial waves were neglected in the calculations [17]. Note that the total angular momentum and parity, as well as isospin and its projection for 3H are given by $\frac{1}{2}^+, \frac{1}{2}, \frac{1}{2}$ respectively. Thus the states $\{3\}S$, $\{21\}D$ and $\{21\}S$ that were mentioned are of the form (17.34) where S and D correspond to $\Lambda = 0$ and 2, while $J = \frac{1}{2}, T = \frac{1}{2}, M_T = \frac{1}{2}$.

The results of these calculations [17] are presented in Table III.1.

It should be noted that the resulting binding energy 6.30 MeV is comparable with the results obtained for the Hamada-Johnston potential in ref. [19] [$B_T = (5.8 \pm 0.5)$ MeV] and ref. [20] [$B_T = (6.5 \pm 1.0)$ MeV], using the usual Rayleigh-Ritz variational principle. The result of Jackson *et al.*

[17] is also in agreement with the calculations of Tjon *et al.* [21] for the Reid potential by the Faddeev's method [$B_T = (6.5 \pm 0.25)$ MeV].

Jackson *et al.* [17] investigated various ways of extrapolation and have found that in the limit of infinite number of quanta their calculation would give the binding energy [$B_T = (6.50 \pm 0.08)$ MeV].

The difference between theoretical and experimental (8.48 MeV) triton binding energy can be connected [22,23] with a contribution of three-body forces or with non-adequate off-shell behavior of two-body T -matrix for the Reid potential. As it was mentioned by Jackson *et al.* [22] the relativistic effect can not change this discrepancy more than 0.25 MeV.

It is possible to conclude that the three-body calculations, using the harmonic oscillator basis, can give the precision comparable with the bests variational calculations even for the realistic potentials with a strong repulsive core.

It is important to note that the procedure of Jackson *et al.* [17], giving the triton ground state wave function, can be modified very easily to produce the ${}^3\text{He}$ ground state wave function.

b) Form factors of ${}^3\text{H}$ and ${}^3\text{He}$

The general formula of the form factor for any nucleus is given in Eq. (19.12) where $f_1(q), f_o(q)$ are respectively the form factors of proton and neutron known experimentally and $F_\nu(q), \nu = 0, 1$ is the contribution of the state of the nucleus for the proton and neutron part, and was obtained in (19.15). Thus all we need is to propose the combination of appropriate orbital and spin isospin states of three-body systems, with harmonic oscillator interactions, that are translationally invariant, and introduce them in (19.15).

For the orbital part, these states corresponding to a definite irreducible representation f of the permutation group of three particles and Yamanouchi symbol r are given in Section 17, while for the spin-isospin part the construction is elementary [24], and they can be denoted by

$$|SM_S, T = \frac{1}{2} M_T, \tilde{f}\tilde{r}\rangle; \quad (20.3)$$

as the isospin for ${}^3\text{H}, {}^3\text{He}$ is $1/2$ and its projection $M_T = (1/2)(3 - 2Z)$ is respectively $(1/2), (-1/2)$. The \tilde{f}, \tilde{r} are the partition and Yamanouchi symbols associated with f, r , as indicated at the end of Section 17. The spin is $S = 1/2$ or $3/2$ and it should combine with the orbital angular momenta Λ in such a way that the total angular momentum $J = 1/2$, as required by the ground states of ${}^3\text{H}$ or ${}^3\text{He}$.

From (17.32) we note that the type of matrix elements that we have to deal with in the orbital part can all be reduced to the form

$$\begin{aligned} & \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \Lambda M_\Lambda | \frac{\sin \kappa |\dot{x}_2|}{\kappa |\dot{x}_2|} | \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \Lambda M_\Lambda \rangle \\ &= \left[\int_0^\infty R_{\dot{n}'_2 \dot{l}'_2}(r) R_{\dot{n}_2 \dot{l}_2}(r) (\kappa r)^{-1} (\sin \kappa r) r^2 dr \right] \delta_{\dot{n}'_1 \dot{n}_1} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{l}'_2 \dot{l}_2}, \\ &= \left[\sum_p B(\dot{n}'_2 \dot{l}_2, \dot{n}_2 \dot{l}_2, p) I_p(\kappa^2) \right] \delta_{\dot{n}'_1 \dot{n}_1} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{l}'_2 \dot{l}_2}, \end{aligned} \quad (20.4)$$

with the Talmi integral $I_p(\kappa^2)$ given by (2.7) in which we replaced $f(r)$ by $(\kappa r)^{-1} \sin \kappa r$ and the $B(n'l', nl, p)$ is defined in (2.6) and tabulated in ref. [7]. For the operator $(\kappa r)^{-1} \sin \kappa r$ of the form factor the Talmi integrals can be given explicitly in terms of Hermite polynomials as [25]

$$\begin{aligned} I_p &= 2 \left[\Gamma\left(p + \frac{3}{2}\right) \right]^{-1} \int_0^\infty r^{2p} e^{-r^2} (\kappa r)^{-1} (\sin \kappa r) r^2 dr \\ &= e^{-\kappa^2/4} (-1)^p (p!) \left[(2p+1)! \right]^{-1} \kappa^{-1} H_{2p+1}(\kappa/2). \end{aligned} \quad (20.5)$$

For the spin-isospin matrices we need in (19.15) the elements

$$\langle SM_S, T = \frac{1}{2} M_T, \tilde{f}'\tilde{r}' | \frac{1}{2} + (-1)^\nu t_{03} | SM_S, T = \frac{1}{2} M_T, \tilde{f}\tilde{r} \rangle, \quad (20.6)$$

and they were calculated in reference [26].

Thus we can proceed to determine explicitly the form factors of ${}^3\text{H}, {}^3\text{He}$ once we specify the combination of orbital states of the form discussed in Section 17, that we want to use as a model of the ground state orbital wave function for ${}^3\text{H}$ and ${}^3\text{He}$. The oscillator states we have to deal with will all have the form (17.32) and we begin with the ground state

$$|00, 00, 00\{3\}\rangle = |\ddot{0}\ddot{0}, \ddot{0}\ddot{0}, 00\rangle, \quad (20.7)$$

where the dotted ones imply the dependence on the Jacobi coordinates (17.3) with $\dot{n}_1 = \dot{l}_1 = \dot{n}_2 = \dot{l}_2 = 0$. The fully antisymmetric oscillator ground state function including the spin-isospin part has then the form

$$|\mathcal{S}\rangle = |\ddot{0}\ddot{0}, \ddot{0}\ddot{0}, 00\rangle | \frac{1}{2} M_S, \frac{1}{2} M_T, \{111\} \rangle, \quad (20.8)$$

where we call it $|\mathcal{S}\rangle$ to stress the total orbital angular momentum 0. We can add innumerable excited states to that in Eq. (20.8), with appropriate coefficients, but recent work [23] suggests that the main contribution will be that of a \mathcal{D} state *i.e.*, $\Lambda = 2$ with partition $\{21\}$. The one with the lowest number of oscillator quanta will, in the notation (17.32), be

$$|02, 00, 2M_\Lambda; \{21\}r\rangle. \quad (20.9)$$

To give a total angular momentum $J = 1/2$, it can only be combined with the spin-isospin

$$|S = \frac{3}{2}M_S, T = \frac{1}{2}M_T, \{21\}\tilde{r}\rangle, \quad (20.10)$$

and using (17.32) to express the full antisymmetric ket, which we denote by $|\mathcal{D}\rangle$, i.e., $\Lambda = 2$, we can write it as

$$\begin{aligned} |\mathcal{D}\rangle = \frac{1}{\sqrt{2}} & \left\{ \frac{1}{\sqrt{2}} \left[|0\dot{0}, \dot{0}2, 2M_\Lambda\rangle |0\dot{2}, \dot{0}0, 2M_\Lambda\rangle \right] | \frac{3}{2}M_S, \frac{1}{2}M_T, \{21\}2 \rangle \right. \\ & \left. - |0\dot{1}, \dot{0}1, 2M_\Lambda\rangle | \frac{3}{2}M_S, \frac{1}{2}M_T, \{21\}1 \rangle \right\}, \end{aligned} \quad (20.11)$$

where the Yamanouchi symbols 211 and 121 are replaced by the notation 1 and 2, and for the calculation of the form factor (19.15) we do not need to couple them to the definite angular momentum $J = 1/2$.

We now proceed to do our calculation in the simplest possible way by assuming the neutron and proton are point particles so $f_1 = 1, f_o = 0$ and thus we are interested only in $F_\nu(q^2)$ with $\nu = 1$ and we use as our state the combination

$$\cos \delta |S\rangle + \sin \delta |\mathcal{D}\rangle. \quad (20.12)$$

All the matrix elements we require have been given above or in [26] and thus, after elementary computations, we arrive at the following form factors for the nuclei we are interested in

$$F_1(\kappa^2) = [1 - (1/6)\kappa^2 \sin^2 \delta] e^{-\kappa^2/4}, \text{ for } {}^3\text{H}, \quad (20.13a)$$

$$F_1(\kappa^2) = [1 - (1/6)\kappa^2 \sin^2 \delta + (1/60)\kappa^4 \sin^2 \delta] e^{-\kappa^2/4}, \text{ for } {}^3\text{He}, \quad (20.13b)$$

where $\cos \delta$ appears only squared so we could replace it by $1 - \sin^2 \delta$.

Note that we have the parameter $\sin^2 \delta$ in our form factors and we could use it to give the best fit to the experimental results. Furthermore from the relation (19.17), which in our case turns out to be

$$\kappa = q \left(\frac{2}{3} \frac{\hbar}{m\omega} \right)^{1/2}, \quad (20.14)$$

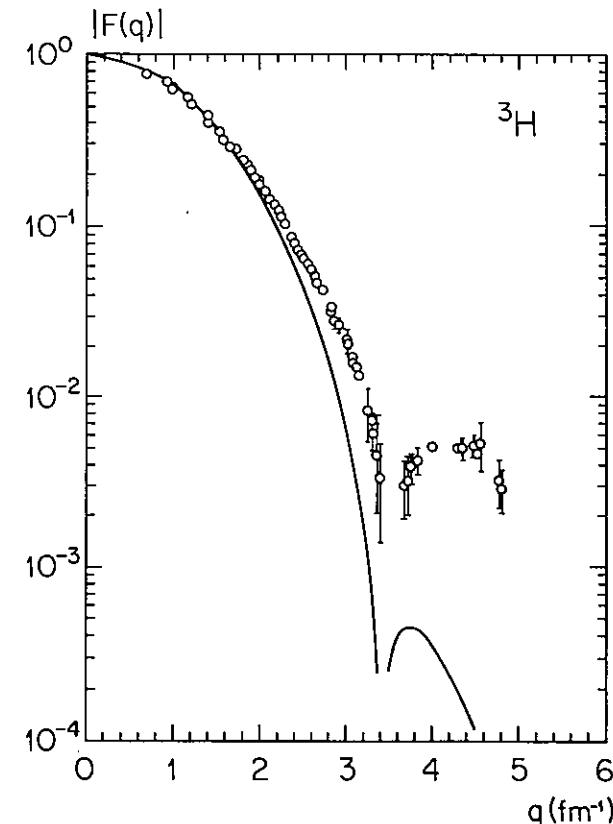


Figure III.1. The charge form factor of ${}^3\text{H}$. The open circles present the experimental data taken from the survey in ref. [23]. The solid curve corresponds to the Eq. (20.13a) with parameters given in the text.

we can express the form factor in terms of q , which is the momentum transfer in units fm^{-1} .

For brevity we shall discuss only the form factor of ${}^3\text{H}$ and adjust the frequency ω of the oscillator and the parameter $\sin^2 \delta$ to fit the radius 1.76 fm [23] of this nucleus, and get the dip of the form factor at the right value of q .

For comparison with experiment in Fig. III.1 we used $\sin^2 \delta = 0.3$ and (in ordinary units) $(\hbar/m\omega) = 2.58 \text{ fm}^2$. We note that the value of $\sin^2 \delta$ is high, but it confirms [23] the importance of the $|\mathcal{D}\rangle$ ket in the ground state of ${}^3\text{H}$. The fit is quite good for low values of q , but the secondary maximum is too low reflecting the simplicity of our wave function.

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Chapter IV

The Four-Body Problem

In this chapter we would like to repeat for the four-particle problem the general discussion we gave for the three-particle problem in the previous chapter and then analyze applications to specific cases such as the α particle.

The matrix elements of the Hamiltonian for translationally invariant states and the nuclear form factor were discussed in chapter III for an arbitrary number of particles; as a result, the only new material we need is the determination of both the translationally invariant and general four-particle harmonic oscillator states. This means extending (done by Aguilera-Navarro, Kramer and Moshinsky, *Ann. Phys., N. Y.*, **54**, 379 (1969)) to four particles the material discussed in sections 17 and 18. While this can be done as fully as for the three-particle problem it is lengthy and besides the general ideas are similar. We shall therefore in this chapter concentrate on a specific problem: the determination of translationally invariant four-particle harmonic oscillator states that are symmetric under exchange of the coordinates and have zero orbital angular momentum. These states will then be used for the discussion of the form factor of the ground state of the α particle.

This specific problem will illustrate all the new concepts we need to generalize to four particles the reasoning carried for three in sections 17 and 18.

As a first step in the construction of the symmetric states of zero orbital angular momentum, we introduce a convenient symmetrical set of relative coordinates for the four-particle system, which we proceed to define and use in the next section.

21 Harmonic Oscillator States in the Symmetrical System of Relative Coordinates

From (16.2) the Jacobi relative coordinates of the four-particle system are given by

$$\left. \begin{aligned} \dot{\mathbf{x}}_1 &= \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2), \\ \dot{\mathbf{x}}_2 &= \frac{1}{\sqrt{6}}(\mathbf{x}_1 + \mathbf{x}_2 - 2\mathbf{x}_3), \\ \dot{\mathbf{x}}_3 &= \frac{1}{\sqrt{12}}(\mathbf{x}_1 + \mathbf{x}_2 + \mathbf{x}_3 - 3\mathbf{x}_4). \end{aligned} \right\} \quad (21.1)$$

The corresponding single coordinate states are $\langle \dot{\mathbf{x}}_s | n_s l_s m_s \rangle$, $s = 1, 2, 3$. A wave function of zero total orbital angular momentum in the three coordinates is then given by the ket

$$\begin{aligned} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2; \dot{n}_3 \dot{l}_3\rangle &\equiv |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2 (L' = l_3); \dot{n}_3 \dot{l}_3, L = 0\rangle \\ &= \left[[\langle \dot{\mathbf{x}}_1 | \dot{n}_1 \dot{l}_1 \rangle \langle \dot{\mathbf{x}}_2 | \dot{n}_2 \dot{l}_2 \rangle]_{L'=l_3} \langle \dot{\mathbf{x}}_3 | \dot{n}_3 \dot{l}_3 \rangle \right]_{L=0}, \end{aligned} \quad (21.2)$$

where, as before, the square brackets represent vector couplings.

In a similar fashion we define the states

$$|\dot{n}_1 \dot{l}_1; \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3\rangle, \quad (21.3)$$

in which the last two particles are coupled to angular momentum $L' = l_1$, and then coupled with the first particle to $L = 0$. The states (21.2) can be decomposed in terms of the states (21.3) or viceversa with the help of Racah coefficients [1]. It is easily seen, though, that because $L = 0$, there is only one term in the expansion with coefficient unity, so (21.2) and (21.3) are identical; when convenient, we shall use for them the generic notation

$$|\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3\rangle, \quad (21.4)$$

where the absence of the semicolon indicates that the order in which we do the coupling is irrelevant. It is, however, important to note that in (21.4) the first set of quantum numbers belongs to coordinate $\dot{\mathbf{x}}_1$, the second to $\dot{\mathbf{x}}_2$, and the third to $\dot{\mathbf{x}}_3$. Thus in (21.4) $(\dot{n}_2 \dot{l}_2)$ belongs to $\dot{\mathbf{x}}_2$, and $(\dot{n}_3 \dot{l}_3)$ to $\dot{\mathbf{x}}_3$, while in $|\dot{n}_1 \dot{l}_1, \dot{n}_3 \dot{l}_3, \dot{n}_2 \dot{l}_2\rangle$ it is the other way around.

The construction of translationally invariant harmonic oscillator states of four particles with $L = 0$, depending on the Jacobi coordinates $\dot{\mathbf{x}}_s$, $s =$

1, 2, 3, is then trivial. What is less trivial is to find out linear combinations of them that have a definite permutational symmetry and, in particular, those that are completely symmetrical under the exchange of the coordinates of the four particles.

It turns out that the construction of these symmetrical states can be achieved much more simply if instead of starting with the Jacobi relative coordinates (21.1) we define the symmetrical relative coordinates

$$\left. \begin{aligned} \ddot{\mathbf{x}}_1 &= \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_4 - \mathbf{x}_2 - \mathbf{x}_3), \\ \ddot{\mathbf{x}}_2 &= \frac{1}{2}(\mathbf{x}_2 + \mathbf{x}_4 - \mathbf{x}_1 - \mathbf{x}_3), \\ \ddot{\mathbf{x}}_3 &= \frac{1}{2}(\mathbf{x}_3 + \mathbf{x}_4 - \mathbf{x}_1 - \mathbf{x}_2). \end{aligned} \right\} \quad (21.5)$$

related to the Jacobi coordinates by the orthogonal transformation

$$\begin{pmatrix} \ddot{\mathbf{x}}_1 \\ \ddot{\mathbf{x}}_2 \\ \ddot{\mathbf{x}}_3 \end{pmatrix} = \mathbf{M} \begin{pmatrix} \dot{\mathbf{x}}_1 \\ \dot{\mathbf{x}}_2 \\ \dot{\mathbf{x}}_3 \end{pmatrix}, \quad \mathbf{M} = \|M_{st}\| = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{3}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{3}} \\ 0 & -\sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} \end{pmatrix}. \quad (21.6)$$

We could also define our single-particle states in terms of the coordinates $\ddot{\mathbf{x}}_s$, $s = 1, 2, 3$, and from them, exactly in the same way as in (21.2), we get the ket

$$|n_1 l_1, n_2 l_2; n_3 l_3\rangle = \left[[\langle \ddot{\mathbf{x}}_1 | n_1 l_1 \rangle \langle \ddot{\mathbf{x}}_2 | n_2 l_2 \rangle]_{l_3} \langle \ddot{\mathbf{x}}_3 | n_3 l_3 \rangle \right]_0, \quad (21.7)$$

which we distinguish from the same ket for the Jacobi coordinates by a final round bracket) rather than by the angular one).

We shall proceed to show that the effect of a permutation of the coordinates \mathbf{x}_s , $s = 1, 2, 3, 4$, on the states (21.7) is very simple to obtain, so that a symmetrical state or, in fact, a state with arbitrary permutational symmetry, is easily determined.

Let us first see what is the effect of any element of the symmetric group $S(4)$ of permutations of the \mathbf{x}_s on the coordinates (21.5). For the symmetrical coordinates $\ddot{\mathbf{x}}_s$, $s = 1, 2, 3$, it is clearly enough to apply the generators of the $S(4)$ group, which we could choose as the transposition (1,2), (2,3), (3,4). We obtain then

$$(1, 2) \begin{pmatrix} \ddot{\mathbf{x}}_1 \\ \ddot{\mathbf{x}}_2 \\ \ddot{\mathbf{x}}_3 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \ddot{\mathbf{x}}_1 \\ \ddot{\mathbf{x}}_2 \\ \ddot{\mathbf{x}}_3 \end{pmatrix},$$

$$(2, 3) \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix},$$

$$(3, 4) \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix}$$

$$= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \end{pmatrix}. \quad (21.8)$$

We immediately see that the subgroup of permutations $S(3)$ of $S(4)$, that permutes $x_s, s = 1, 2, 3$, does just exactly the same thing for $\ddot{x}_s, s = 1, 2, 3$. On the other hand, the invariant subgroup $D(2)$ of $S(4)$, consisting of the permutations

$$D(2) : e, d_1 = (2, 3)(1, 4), d_2 = (1, 3)(2, 4), d_3 = (1, 2)(3, 4), \quad (21.9)$$

has, from (21.8), the following representation when acting on the vector whose three components are $\ddot{x}_s, s = 1, 2, 3$:

$$D(2) : e = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad d_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix};$$

$$d_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}; \quad d_3 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (21.10)$$

The group $S(4)$ can be expressed as a semidirect product [2] of these two subgroups:

$$S(4) = D(2) \wedge S(3); \quad (21.11)$$

this implies that any element ρ of $S(4)$ can be expressed in a unique way as the product

$$\rho = dp, \quad (21.12)$$

with d an element of $D(2)$ and p an element of $S(3)$. Therefore the projection operator \mathcal{P} for a symmetric state of the four-particle system takes the form

$$\mathcal{P} = \sum_{\rho} \rho = \sum_p (e + d_1 + d_2 + d_3)p. \quad (21.13)$$

The application of the projection operator \mathcal{P} to the states $|n_1 l_1, n_2 l_2, n_3 l_3\rangle$ is now very simple: we must apply, in succession, the reciprocals of all

elements ρ to the coordinates \ddot{x}_s in the ket. As from (21.12) and (21.10) $\rho^{-1} = p^{-1}d^{-1} = p^{-1}d$, we first apply the sum of the four elements between parentheses of (21.13) to the ket (21.7); this gives

$$(e + d_1 + d_2 + d_3)|n_1 l_1, n_2 l_2, n_3 l_3\rangle = [1 + (-1)^{l_2+l_3} + (-1)^{l_1+l_3} + (-1)^{l_1+l_2}]|n_1 l_1, n_2 l_2, n_3 l_3\rangle. \quad (21.14)$$

The effect of (1,2) on the ket (21.7) is

$$(1, 2)|n_1 l_1, n_2 l_2, n_3 l_3\rangle = (-1)^{l_1+l_2-l_3}|n_2 l_2, n_1 l_1, n_3 l_3\rangle, \quad (21.15)$$

while for the same reason, the effect of (2,3) on the ket $|n_1 l_1, n_2 l_2, n_3 l_3\rangle$ is

$$(2, 3)|n_1 l_1, n_2 l_2, n_3 l_3\rangle = (-1)^{l_2+l_3-l_1}|n_1 l_1, n_3 l_3, n_2 l_2\rangle. \quad (21.16)$$

Now the semicolon can be suppressed because the order of the coupling is irrelevant; moreover, the $l_s, s = 1, 2, 3$, are integers; so we see that the effect of a permutation of $S(3)$ on $|n_1 l_1, n_2 l_2, n_3 l_3\rangle$ is to permute the indices $n_s l_s$, giving an extra factor $(-1)^{l_1+l_2+l_3}$ if the permutation is odd and no factor if it is even. Thus the application of the projection operator \mathcal{P} to the ket (21.7) leads to the state

$$\begin{aligned} \mathcal{P}|n_1 l_1, n_2 l_2, n_3 l_3\rangle = & [1 + (-1)^{l_2+l_3} + (-1)^{l_1+l_3} + (-1)^{l_1+l_2}] \\ & \times \{[|n_1 l_1, n_2 l_2, n_3 l_3\rangle + |n_2 l_2, n_3 l_3, n_1 l_1\rangle + |n_3 l_3, n_1 l_1, n_2 l_2\rangle] \\ & + (-1)^{l_1+l_2+l_3} [|n_2 l_2, n_1 l_1, n_3 l_3\rangle + |n_3 l_3, n_2 l_2, n_1 l_1\rangle \\ & + |n_1 l_1, n_3 l_3, n_2 l_2\rangle]\}. \end{aligned} \quad (21.17)$$

For the particular case of the ground state of the α particle, the parity is positive. As the parity of the state (21.7) is $(-1)^{l_1+l_2+l_3}$, we conclude that we are only interested in states in which $l_1 + l_2 + l_3$ is even. This can only be achieved if either all l_s are even or if two of them are odd. But the second case is uninteresting, because the first square bracket in the symmetrised state (21.17) will be zero. Therefore, we need only concern ourselves with the normalized state projected from $|n_1 l_1, n_2 l_2, n_3 l_3\rangle$ when l_1, l_2, l_3 are even; that is to say, with

$$\begin{aligned} |n_1 l_1, n_2 l_2, n_3 l_3\rangle_S \equiv A & [|n_1 l_1, n_2 l_2, n_3 l_3\rangle + |n_1 l_1, n_3 l_3, n_2 l_2\rangle \\ & + |n_2 l_2, n_3 l_3, n_1 l_1\rangle + |n_2 l_2, n_1 l_1, n_3 l_3\rangle \\ & + |n_3 l_3, n_1 l_1, n_2 l_2\rangle + |n_3 l_3, n_2 l_2, n_1 l_1\rangle]. \end{aligned} \quad (21.18)$$

The normalization constant A is $1/\sqrt{6}$ if all three pairs $n_s l_s$ are distinct, $1/\sqrt{12}$ if any two pairs are equal, and $1/6$ if all pairs are equal.

We have constructed explicitly the nonspurious, *i.e.*, translationally invariant harmonic oscillator states of a four-particle system that are symmetric under exchange of the coordinates, and whose total orbital angular momentum is zero. These states are expressed in terms of the symmetrical coordinates $\ddot{x}_s, s = 1, 2, 3$. For the calculation of the form factor (19.21), as well as for the matrix elements of the intrinsic Hamiltonian (16.11), we need to express these states in terms of those in the Jacobi coordinates $\dot{x}_s, s = 1, 2, 3$. We proceed to do this in the next section.

22 Transformation Brackets Between the States in the Symmetrical and Jacobi Coordinate Systems

Using the notation $| \rangle$ and $\langle |$ for the states of coordinates $\ddot{x}_s, \dot{x}_s, s = 1, 2, 3$, respectively, we can carry out the expansion

$$|n_1 l_1, n_2 l_2, n_3 l_3\rangle = \sum_{\dot{n}_s, \dot{l}_s} |\dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3\rangle \langle \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3 | n_1 l_1, n_2 l_2, n_3 l_3 \rangle, \quad (22.1)$$

where the brackets $\langle |$) are those we want to determine. We note that the total orbital angular momentum L is zero both in $| \rangle$ and $\langle |$ states; in fact we have

$$\begin{aligned} L_i &\equiv \sum_{s=1}^3 \sum_{j,k=1}^3 \epsilon_{ijk} \ddot{x}_{js} \ddot{p}_{ks} \\ &= \sum_{r,s,t=1}^3 \sum_{j,k=1}^3 \epsilon_{ijk} M^{st} \dot{x}_{ji} M^{sr} \dot{p}_{kr} \\ &= \sum_{t=1}^3 \sum_{j,k=1}^3 \epsilon_{ijk} \dot{x}_{jt} \dot{p}_{kt} \\ &\equiv \dot{L}_i, \end{aligned} \quad (22.2)$$

because $\|M_{st}\|$ of (21.6) is an orthogonal matrix. Furthermore, the summation in (22.1) involve only a finite number of terms because, for the same reasons as in (22.2), we have

$$H \equiv \frac{1}{2} \sum_{s=1}^3 \left[(\ddot{p}_s)^2 + (\ddot{x}_s)^2 \right] = \frac{1}{2} \sum_{s=1}^3 \left[(\dot{p}_s)^2 + (\dot{x}_s)^2 \right] \equiv \dot{H}, \quad (22.3)$$

22. TRANSFORMATION BRACKETS

so that

$$2n_1 + l_1 + 2n_2 + l_2 + 2n_3 + l_3 = 2\dot{n}_1 + \dot{l}_1 + 2\dot{n}_2 + \dot{l}_2 + 2\dot{n}_3 + \dot{l}_3, \quad (22.4)$$

and all the quantum numbers are non negative integers.

To obtain the explicit form of the transformation brackets we first note that M of (21.6) could be written as

$$\begin{aligned} M &= \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} \\ 0 & -\sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \\ &\equiv M_1 M_2 M_3, \end{aligned} \quad (22.5)$$

where $M_\alpha, \alpha = 1, 2, 3$, is the notation we shall use when we refer to the three matrices in (22.5) in the order indicated.

Now it is clear that the effect of the transformation M_3 on a state $|n_1 l_1, n_2 l_2, n_3 l_3\rangle$ is just to multiply it by the phase factor $(-1)^{l_3}$, since this matrix is diagonal.

To see the effect of the transformation M_1 we first interpret the state as

$$|n_1 l_1, n_2 l_2, n_3 l_3\rangle = |n_1 l_1, n_2 l_2 (L' = l_3); n_3 l_3; L = 0\rangle. \quad (22.6)$$

Clearly M_1 affects (22.6) in the same way as a rotation through an angle $\frac{1}{2}\beta = \frac{1}{4}\pi$ in the space of the first two coordinates; in other words, it is equivalent to the transformation

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix} \quad (22.7)$$

acting on the two-particle state

$$|n_1 l_1, n_2 l_2, l_3 m_3\rangle \quad (22.8)$$

of total angular momentum l_3 . As was shown in section 10, the transformation (22.7) gives rise to the standard transformation brackets

$$\langle n_l, NL, l_3 | n_1 l_1, n_2 l_2, l_3 \rangle \quad (22.9)$$

tabulated by Brody and Moshinsky [3], which we shall employ to determine the effect of M_1 on the states (22.6).

If we write our state as

$$|n_1 l_1, n_2 l_2, n_3 l_3\rangle = |n_1 l_1; n_2 l_2, n_3 l_3 (L' = l_1); L = 0\rangle, \quad (22.10)$$

it becomes clear that M_2 affects (22.10) in the same way as a rotation through an angle $\frac{1}{2}\beta$ such that $\cos \frac{1}{2}\beta = 1/\sqrt{3}$, it i.e., $\beta = 109.47^\circ$, in the space of coordinates 2 and 3; the equivalent transformation is

$$\begin{pmatrix} x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{2}{3}} \\ -\sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \end{pmatrix} \begin{pmatrix} x \\ X \end{pmatrix} \quad (22.11)$$

acting on the two-particle state

$$|n_2 l_2, n_3 l_3, l_1 m_1\rangle \quad (22.12)$$

of total angular momentum l_1 . This would give rise to transformation brackets of the type (22.9), but for a rotation angle $\frac{1}{2}\beta$ instead of $\pi/4$; these we have designated by

$$\langle nl, NL, l_1 | n_2 l_2, n_3 l_3, l_1 \rangle_\beta. \quad (22.13)$$

In section 15 we discussed Gal's demonstration [4] that these transformation brackets may be written in terms of sums of products of two standard transformation brackets [3] of the type (22.9), and phase factors depending on β . It is clear therefore that the transformation brackets $\langle \rangle$ in (22.1) can be obtained straightforwardly in terms of the tabulated [3] brackets (22.9).

In the next section we apply the procedure outlined here to give the transformation brackets $\langle \rangle$ for even parity states of up to four quanta.

23 Form Factor for a Linear Combination of Harmonic Oscillator States. Application to the α Particle

We shall proceed to discuss the symmetrized states $|n_1 l_1, n_2 l_2, n_3 l_3\rangle_S$ of (21.18), with l_1, l_2, l_3 even, when the total number of quanta

$$\mathfrak{N} = 2n_1 + l_1 + 2n_2 + l_2 + 2n_3 + l_3 \quad (23.1)$$

takes all even values up to $\mathfrak{N} = 4$.

For $\mathfrak{N} = 0$ all quantum numbers must be zero, and our first state which we designate by $|1\rangle$ becomes

$$|1\rangle \equiv |00, 00, 00\rangle_S = |00, 00, 00\rangle. \quad (23.2)$$

For $\mathfrak{N} = 2$ we may have either $n_1 = 1$ and all the other quantum numbers zero, or else $l_1 = l_2 = 1$ and the remainder zero; and the permutations of these two possibilities. However, the second one may be eliminated, because as we have seen, l_1 and l_2 may not be odd. So we are left with only one state, which we shall write as

$$|2\rangle = |10, 00, 00\rangle_S. \quad (23.3)$$

For $\mathfrak{N} = 4$ and $l_1 l_2 l_3$ even we have, apart from permutations, only the following three choices for the angular momenta: (000), (200) and (220). The second possibility has to be eliminated, because the corresponding state would then have a total angular momentum $L = 2$ and not zero as required. For (000) we can have either $n_1 = 2, n_2 = n_3 = 0$ or $n_1 = n_2 = 1, n_3 = 0$ and, of course, the permutations of these choices. For (220) and $\mathfrak{N} = 4$ we must take $n_1 = n_2 = n_3 = 0$. We thus have only three possible states of 4 quanta:

$$\left. \begin{array}{l} |3\rangle \equiv |20, 00, 00\rangle_S, \\ |4'\rangle \equiv |10, 10, 00\rangle_S, \\ |5'\rangle \equiv |02, 02, 00\rangle_S. \end{array} \right\} \quad (23.4)$$

For convenience in later numerical calculations, instead of $|4'\rangle$ and $|5'\rangle$, we use an orthogonal transformation of these given by

$$\left. \begin{array}{l} |4\rangle = \frac{\sqrt{5}}{3}|4'\rangle + \frac{2}{3}|5'\rangle, \\ |5\rangle = \frac{2}{3}|4'\rangle - \frac{\sqrt{5}}{3}|5'\rangle. \end{array} \right\} \quad (23.5)$$

We proceed now to use the analysis given in section 22 to rewrite these states in terms of those expressed in Jacobi coordinates, and we find, in a straightforward fashion that

$$|1\rangle = |00, 00, 00\rangle \quad (23.6a)$$

$$|2\rangle = \frac{1}{\sqrt{3}}[|10, 00, 00\rangle + |00, 10, 00\rangle + |00, 00, 10\rangle] \quad (23.6b)$$

$$\begin{aligned} |3\rangle &= \frac{1}{\sqrt{12}}[|20, 00, 00\rangle + |00, 20, 00\rangle \\ &\quad + \frac{2}{3}|00, 00, 20\rangle] - \frac{\sqrt{10}}{9}|10, 01, 01\rangle \\ &\quad + \frac{\sqrt{10}}{18}[|10, 10, 00\rangle \end{aligned}$$

$$\begin{aligned}
& + 2|00,10,10\rangle + 2|10,00,10\rangle] - \frac{2\sqrt{2}}{9}|02,01,01\rangle \\
& + \frac{\sqrt{2}}{9}|[02,02,00\rangle \\
& + 2|00,02,02\rangle + 2|02,00,02\rangle] + \frac{\sqrt{6}}{9}|00,11,01\rangle \quad (23.6c)
\end{aligned}$$

$$\begin{aligned}
|4\rangle &= \frac{1}{2\sqrt{2}}[|20,00,00\rangle + |00,20,00\rangle \\
& + \frac{4}{3}|00,00,20\rangle] + \frac{1}{6}\sqrt{\frac{5}{3}}|10,10,00\rangle \\
& + \frac{1}{3\sqrt{3}}|02,02,00\rangle + \frac{1}{3}\sqrt{\frac{5}{3}}|10,01,01\rangle \\
& + \frac{2}{3\sqrt{3}}|02,01,01\rangle - \frac{1}{3}|00,11,01\rangle \quad (23.6d)
\end{aligned}$$

$$\begin{aligned}
|5\rangle &= \frac{2}{3\sqrt{3}}[|10,10,00\rangle + |10,00,10\rangle + |00,10,10\rangle] \\
& - \frac{1}{3}\sqrt{\frac{5}{3}}[|02,02,00\rangle + |02,00,02\rangle + |00,02,02\rangle]. \quad (23.6e)
\end{aligned}$$

We designate the states (23.6) generically by $|m\rangle$, $m = 1, 2, 3, 4, 5$. If we limit ourselves to $\mathfrak{N} \leq 4$, the most general symmetrical translationally invariant four-particle state of zero orbital angular momentum and even parity is given by

$$\sum_{m=1}^5 a_m |m\rangle, \quad (23.7)$$

where a_m are the, as yet, undetermined coefficients in the expansion.

If the wave function (23.7) represents the ground state of the α particle for which $n = 4$, $Z = 2$ the corresponding neutron and proton distribution form factors given by (19.21) are equal; we call them both $F(q^2)$ and rewrite (19.21) as

$$F(q^2) = \sum_{m'm} \langle m' \left| \frac{\sin \kappa |\dot{x}_3|}{\kappa |\dot{x}_3|} \right| m \rangle a_{m'}^* a_m, \quad (23.8)$$

with q^2, κ^2 related as in (19.16).

From (23.6) the matrix elements in (23.8) reduce to linear combinations of

$$\begin{aligned}
& \langle \dot{n}'_1 \dot{l}'_1, \dot{n}'_2 \dot{l}'_2, \dot{n}'_3 \dot{l}'_3 \left| \frac{\sin \kappa |\dot{x}_3|}{\kappa |\dot{x}_3|} \right| \dot{n}_1 \dot{l}_1, \dot{n}_2 \dot{l}_2, \dot{n}_3 \dot{l}_3 \rangle \\
& = \delta_{\dot{n}'_1 \dot{n}_1} \delta_{\dot{l}'_1 \dot{l}_1} \delta_{\dot{n}'_2 \dot{n}_2} \delta_{\dot{l}'_2 \dot{l}_2} \delta_{\dot{l}'_3 \dot{l}_3} \langle \dot{n}'_3 \dot{l}'_3 \left| \frac{\sin \kappa |\dot{x}_3|}{\kappa |\dot{x}_3|} \right| \dot{n}_3 \dot{l}_3 \rangle, \quad (23.9)
\end{aligned}$$

where the last single-body matrix element was evaluated explicitly in (6.6) and (6.7).

Assuming a_m , real we can then write $F(\kappa^2)$ [5] as

$$\begin{aligned}
F(\kappa^2) &= e^{-\frac{1}{4}\kappa^2} \left\{ 1 - \left[\frac{\sqrt{2}}{6} a_1 a_2 + \frac{1}{9} a_2^2 + \frac{\sqrt{5}}{9} a_2 a_3 + \frac{2}{9} \sqrt{\frac{5}{6}} a_2 a_4 \right. \right. \\
& + \frac{2}{9} \sqrt{\frac{2}{3}} a_2 a_5 + \frac{2}{9} (a_3^2 + a_4^2 + a_5^2) \left. \right] \kappa^2 \\
& + \left[\frac{\sqrt{10}}{360} a_1 a_3 + \frac{\sqrt{15}}{180} a_1 a_4 + \frac{1}{72} a_2^2 + \frac{\sqrt{5}}{135} a_2 a_3 + \frac{2}{45} \sqrt{\frac{5}{6}} a_2 a_4 \right. \\
& + \frac{11}{540} a_3^2 + \frac{11}{270} \sqrt{\frac{2}{3}} a_3 a_4 + \frac{1}{135} \sqrt{\frac{10}{3}} a_3 a_5 + \frac{11}{270} a_4^2 + \frac{1}{54} a_5^2 \left. \right] \kappa^4 \\
& - \left[\frac{\sqrt{5}}{2160} a_2 a_3 + \frac{1}{360} \sqrt{\frac{5}{6}} a_2 a_4 + \frac{1}{1620} a_3^2 + \frac{1}{270} \sqrt{\frac{2}{3}} a_3 a_4 \right. \\
& \left. \left. + \frac{1}{270} a_4^2 \right] \kappa^6 + \left[\frac{1}{144} \sqrt{\frac{2}{5}} a_3 + \frac{1}{120} \sqrt{\frac{5}{3}} a_4 \right]^2 \kappa^8 \right\}. \quad (23.10)
\end{aligned}$$

Because of the normalization condition for the wave function,

$$\sum_{m=1}^5 a_m^2 = 1, \quad (23.11)$$

we have only four independent parameters, but this is still too many to plot the variation of F as a function of κ^2 . We must remember also that the frequency of the oscillator is another parameter, as indicated in (19.16).

As a illustration [5] of the behaviour of $|F(\kappa^2)|$ as a function of κ^2 we consider the particular linear combination of states

$$\cos \delta |1\rangle + \sin \delta |4\rangle, \quad -\frac{1}{2}\pi \leq \delta \leq \frac{1}{2}\pi. \quad (23.12)$$

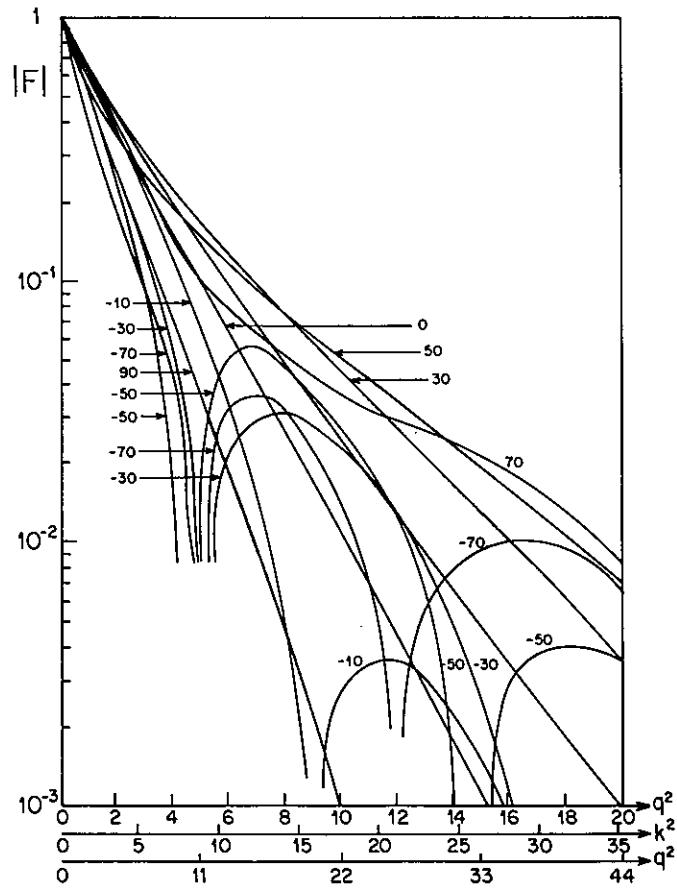


Figure IV.1. Form factor of the α particle as a function of the square of the momentum transfer, when this particle is represented by the non-spurious four-nucleon state (23.12). The curves are characterized by the angles δ with $-\frac{1}{2}\pi \leq \delta \leq \frac{1}{2}\pi$ that give the different mixtures of zero- and four-quantum states. There are three scales in the figure. The middle one is for the dimensionless parameter $\kappa^2 = (2\hbar/3m\omega)q^2$ while the upper and lower ones correspond respectively to q^2 (in fm^{-2}) when $\hbar\omega = 16.8$ and 37 MeV .

23. FORM FACTOR FOR A LINEAR COMBINATION

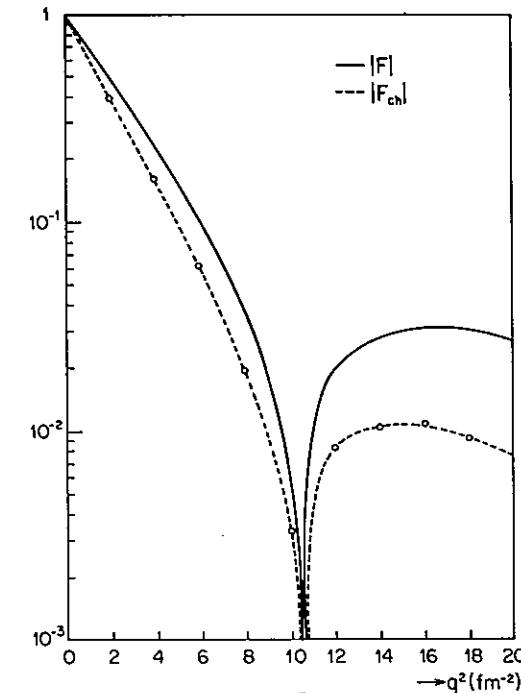


Figure IV.2. Charge form factor (dotted line) of the α particle obtained from the experimental data on electron scattering of reference [7] and the corresponding body form factor (full line) defined in (23.13).

Curves for different values of δ are given in Fig. IV.1, where we use a logarithmic scale for $|F|$. As abscissas we also show the values of q^2 in fm^{-2} obtained from (19.16) for $\hbar\omega = 16.8$ and 37 MeV . We observe for angles such as $\delta = -30^\circ$, -50° or -70° diffraction effects which differ radically from the behaviour of the form factor for the state $|1\rangle$; (23.10) with $a_1 = 1$ and the others zero shows that this is a Gaussian in κ , and so on a logarithmic scale for $|F|$ it would appear as a straight line.

Before comparing $|F(q^2)|$ for certain values of $a_m, m = 1, \dots, 5$, with the experimental results, let us note that from the scattering of high-energy electrons by α particles we get $|F_{ch}(q^2)|$ and not $|F(q^2)|$. But from (19.12) they are related by

$$F_{ch}(q^2) = [f_1(q^2) + f_0(q^2)]F(q^2). \quad (23.13)$$

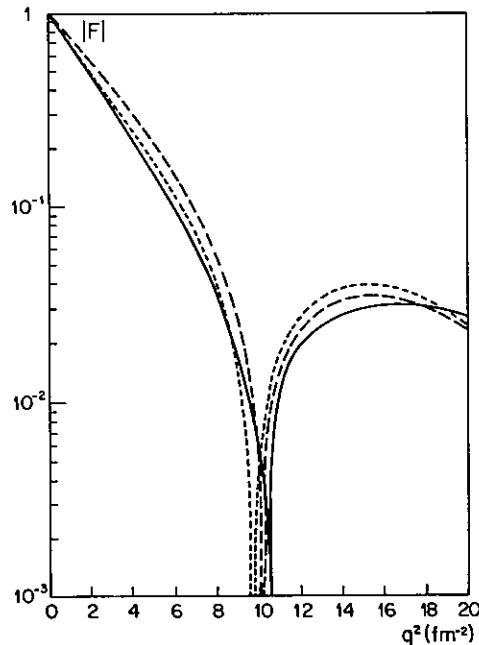


Figure IV.3. Comparison between the experimental body form factor (full line) and the theoretical ones given by (23.10) when we use the state (23.12). The curve of short dashes corresponds to $\delta = -70^\circ$ and $\hbar\omega = 37$ MeV, the curve of long dashes to $\delta = -30^\circ$ and $\hbar\omega = 33.6$ MeV.

Since $f_1(q^2) + f_0(q^2)$, i.e., the sum of the proton and neutron form factors, has been obtained [6] experimentally we may, using (23.13), plot the experimental $|F(q^2)|$ from the $|F_{ch}(q^2)|$ obtained by Frosch [7] *et al.* This is done in Fig. IV.2; the dotted lines gives $|F_{ch}(q^2)|$ and the full line the corresponding $|F(q^2)|$.

Returning now to Fig. IV.1, we observe that for two values of δ , -30° and -70° , the theoretical $F(q^2)$ looks very similar to the experimental one. We corroborate this by drawing all three curves together in Fig. IV.3. Note that the $\hbar\omega$ values that give the best fit for the two values of δ are different.

We have calculated the form factor for the ground state of the α particle for a somewhat arbitrary selection of coefficients $a_m, m = 1, \dots, 5$. A more systematic approach to the determination of these coefficients could be achieved by procedures entirely analogous to those discussed in connection with the electronic form factor of the hydrogen atom in sections 5 and 6.

If we assume a definite intrinsic Hamiltonian for the α particle, then a variational analysis using the state (23.7) and the discussion in sections 16

and 3, would determine both the a_m and the binding energy of the α particle. We must, however, be careful not to use hard-core potentials between the nucleons, for then the matrix elements in section 16 will blow up. Soft-core or velocity-dependent potentials will present no problem.

We could also use a least-squares approach to approximate the experimental values by $F(q^2)$. As shown in section 7, this leads to sets of algebraic equations in the a_m which we could solve by successive approximations until we achieve self-consistency.

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Chapter V

The n -Body Problem in the Hartree–Fock Approximation

The techniques developed in chapters III and IV for the three- and four-body problems could be extended to more particles, but the analytic complications quickly make exact calculations of the matrix elements impracticable. One is therefore forced to consider approximation procedures for many-body calculations among which the Hartree–Fock approximation (HFA) is one of the most widely used. In this chapter we shall use harmonic oscillator states in the systematic application of the Hartree–Fock approximation. Before embarking on this programme, we would like to have some idea of how good the Hartree–Fock approximation is. In the next section we shall use a very simple model [1], again involving harmonic oscillators, to give a critical discussion of the HFA. In the remaining sections of this chapter we discuss the HFA particularly for closed shells, and apply it to some atomic and nuclear problems.

24 How Good Is the Hartree–Fock Approximation? A Simple Model

Consider two particles of equal mass, moving in a common harmonic oscillator well and interacting with each other through a harmonic force of strength κ . The Hamiltonian — in units in which $\hbar = m = \omega = 1$, where ω is the frequency of the common harmonic oscillator well — is

$$H = \frac{1}{2}[(\mathbf{p}_1)^2 + (\mathbf{x}_1)^2 + (\mathbf{p}_2)^2 + (\mathbf{x}_2)^2] + \kappa \left[\frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2) \right]^2. \quad (24.1)$$

Defining relative and centre-of-mass coordinates as in section 10,

$$\mathbf{r} = \frac{1}{\sqrt{2}}(\mathbf{x}_1 - \mathbf{x}_2), \quad \mathbf{R} = \frac{1}{\sqrt{2}}(\mathbf{x}_1 + \mathbf{x}_2), \quad (24.2)$$

and similarly for the momenta, H becomes

$$H = \frac{1}{2}(P^2 + R^2) + \frac{1}{2}[p^2 + (2\kappa + 1)r^2], \quad (24.3)$$

which has the ground state solution, found by standard techniques,

$$\psi = \pi^{-\frac{3}{2}}(2\kappa + 1)^{\frac{3}{8}} \exp(-\frac{1}{2}R^2) \exp(-\frac{1}{2}[2\kappa + 1]^{\frac{1}{2}}r^2). \quad (24.4)$$

The energy (zero quanta) in our units is

$$E = \frac{3}{2}(1 + [2\kappa + 1]^{\frac{1}{2}}). \quad (24.5)$$

So far we have introduced no approximations; (24.4) and (24.5) are exact results. We will now solve the same problem, using the Hartree–Fock analysis, and then compare with (24.4) and (24.5). Assuming that the particles have spin $\frac{1}{2}$ and the same orbital dependence $\phi(\mathbf{x})$, the trial wave function is

$$\begin{aligned} \psi_{HF} \equiv \psi' &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi(\mathbf{x}_1)\chi_{\frac{1}{2}}(1) & \phi(\mathbf{x}_2)\chi_{\frac{1}{2}}(2) \\ \phi(\mathbf{x}_1)\chi_{-\frac{1}{2}}(1) & \phi(\mathbf{x}_2)\chi_{-\frac{1}{2}}(2) \end{vmatrix} \\ &= \phi(\mathbf{x}_1)\phi(\mathbf{x}_2) \frac{1}{\sqrt{2}}[\chi_{\frac{1}{2}}(1)\chi_{-\frac{1}{2}}(2) - \chi_{-\frac{1}{2}}(1)\chi_{\frac{1}{2}}(2)], \end{aligned} \quad (24.6)$$

where, as before, χ_{m_s} is the spin wave function with z -projection $m_s = \pm\frac{1}{2}$. The Hartree–Fock equation for the Hamiltonian (24.1) is

$$\begin{aligned} \frac{1}{2}[(\mathbf{p}_1)^2 + (\mathbf{x}_1)^2]\phi(\mathbf{x}_1) + [\int \phi^*(\mathbf{x}_2)\frac{\kappa}{2}(\mathbf{x}_1 - \mathbf{x}_2)^2\phi(\mathbf{x}_2)d\mathbf{x}_2] \phi(\mathbf{x}_1) \\ = \epsilon\phi(\mathbf{x}_1), \end{aligned} \quad (24.7)$$

where ϵ is to be determined. This is an integrodifferential equation; however, solving it is trivial. Expand $(\mathbf{x}_1 - \mathbf{x}_2)^2$ in the integrand. The term $\int \phi^*(\mathbf{x}_2)\mathbf{x}_1 \cdot \mathbf{x}_2 \phi(\mathbf{x}_2)d\mathbf{x}_2$ vanishes, because of parity. Furthermore,

$$\frac{\kappa}{2} \int \phi^*(\mathbf{r})r^2\phi(\mathbf{r})d\mathbf{r} \equiv A \quad (24.8)$$

is a constant which we may incorporate into ϵ . Eq. (24.7) then becomes

$$\frac{1}{2}[(\mathbf{p}_1)^2 + (\kappa + 1)(\mathbf{x}_1)^2]\phi(\mathbf{x}_1) = \epsilon'\phi(\mathbf{x}_1) = (\epsilon - A)\phi(\mathbf{x}_1), \quad (24.9)$$

where we have also assumed that the ϕ 's are normalised to 1. Eq. (24.9) is easily solved and we find that

$$\phi(r_1) = \pi^{-\frac{3}{4}}(\kappa + 1)^{\frac{3}{8}} \exp[-\frac{1}{2}(1 + \kappa)^{\frac{1}{2}}r_1^2], \quad r_1 \equiv |\mathbf{x}_1|. \quad (24.10)$$

Introducing this into (24.8) and using (24.9), we have

$$\epsilon = \frac{3}{2} \left(\frac{3\kappa + 2}{2\kappa + 2} \right) (\kappa + 1)^{\frac{1}{2}}, \quad (24.11)$$

and

$$\begin{aligned} \psi' &= \phi(r_1)\phi(r_2) = \pi^{-\frac{3}{2}}(1 + \kappa)^{\frac{3}{4}} \exp[-\frac{1}{2}(1 + \kappa)^{\frac{1}{2}}(r_1^2 + r_2^2)] \\ &= \pi^{-\frac{3}{2}}(1 + \kappa)^{\frac{3}{4}} \exp[-\frac{1}{2}(1 + \kappa)^{\frac{1}{2}}(r^2 + R^2)]. \end{aligned} \quad (24.12)$$

This should be compared with the exact result, (24.4).

The Hartree–Fock energy is the expectation value of H with respect to ψ' . Since H can be written in the form

$$H = \frac{1}{2}[(\mathbf{p}_1)^2 + (\kappa + 1)(\mathbf{x}_1)^2] + \frac{1}{2}[(\mathbf{p}_2)^2 + (\kappa + 1)(\mathbf{x}_2)^2] - \kappa\mathbf{x}_1 \cdot \mathbf{x}_2, \quad (24.13)$$

we immediately obtain that the Hartree–Fock energy is

$$E_{HF} \equiv E' = 3 \left[1 + \kappa \right]^{\frac{1}{2}}. \quad (24.14)$$

We may now compare the Hartree–Fock answers with the exact results. For $\kappa = 0$ we have complete agreement, as we expect. In physical applications the interaction potential is usually of the same order of magnitude as the common potential; it is thus of interest to compare the agreement in our model for $\kappa = 1$. In Fig. V.1 we plot the energies of the exact and Hartree–Fock problem as a function of κ . Note that $E < E'$, as it must be. For $\kappa = 1$, E is 96.5% of the Hartree–Fock energy. From (24.4) and (24.12) we see that the overlap $(\psi, \psi')^2$ is given by the expression

$$(\psi, \psi')^2 = \frac{64(\kappa + 1)^{\frac{3}{2}}(2\kappa + 1)^{\frac{3}{4}}}{[1 + \sqrt{(1 + \kappa)}]^3 [\sqrt{(1 + \kappa)} + \sqrt{(1 + 2\kappa)}]^3}, \quad (24.15)$$

which is plotted in Fig. V.2. For $\kappa = 1$ the overlap is about 95%.

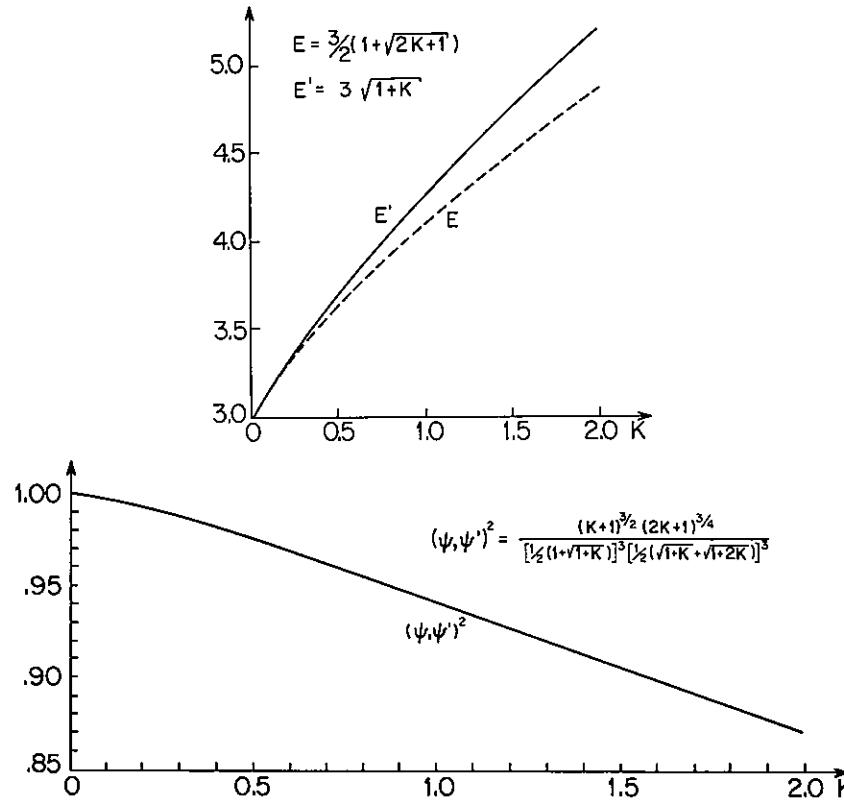


Figure V.1 (top). Exact and Hartree-Fock energies for the two-particle model problem as a function of the coupling parameter κ .

Figure V.2 (bottom). Overlap of the exact and Hartree-Fock wave functions for the two-particle model problem as function of the coupling parameter κ .

Clearly then the Hartree-Fock approximation is, in this simple model, quite good both for the energies and the wave functions.

25 The Set of Algebraic Equations and Their Self-Consistent Solution

The usual atomic or nuclear Hamiltonians can be written in the form

$$H = \sum_{s=1}^n H_0(s) + \sum_{s < t=2}^n V(s, t), \quad (25.1)$$

where $H_0(s)$ is the single-body Hamiltonian for particle s , while $V(s, t)$ is the two-body interaction.

If we are interested only in the expectation value of H with respect to totally antisymmetric wave functions, we may replace H by the operator

$$H' = nH_0(1) + \frac{1}{2}n(n-1)V(1, 2). \quad (25.2)$$

An antisymmetric wave function may be written as the Slater determinant

$$\Psi = \frac{1}{\sqrt{n!}} \det |\psi_i(s)| = \frac{1}{\sqrt{n!}} \epsilon_{i_1 i_2 \dots i_n} \psi_{i_1}(1) \psi_{i_2}(2) \dots \psi_{i_n}(n), \quad (25.3)$$

where repeated indices are summed. In (25.3) $\epsilon_{i_1 i_2 \dots i_n}$ is the totally anti-symmetric tensor defined by

$$\epsilon_{i_1 i_2 \dots i_n} = \begin{cases} +1 & \text{if } i_1 i_2 \dots i_n \text{ is an even permutation of } 1, 2, \dots, n \\ -1 & \text{if } i_1 i_2 \dots i_n \text{ is an odd permutation of } 1, 2, \dots, n \\ 0 & \text{otherwise, i.e., if any two of } i_1 i_2 \dots i_n \text{ are equal.} \end{cases} \quad (25.4)$$

The $\psi_i(s)$ are single-particle states and are assumed orthonormal. The label i may include orbital, spin and isospin quantum numbers.

The expectation value of H with respect to the state (25.3) is then

$$\begin{aligned} (\Psi, H\Psi) &= \frac{n}{n!} \epsilon_{i_1 i_2 \dots i_n} \epsilon_{j_1 j_2 \dots j_n} \int \psi_i^*(1) H_0(1) \psi_j(1) d\tau_1 \\ &\quad + \frac{1}{2} \frac{n(n-1)}{n!} \epsilon_{i_1 i_2 \dots i_n} \epsilon_{k l i_3 \dots i_n} \int \psi_i^*(1) \psi_j^*(2) V(1, 2) \\ &\quad \times \psi_k(1) \psi_l(2) d\tau_1 d\tau_2, \end{aligned} \quad (25.5)$$

where \int may include summations over spins and isospins, and repeated indices are summed from 1 to n .

In the first term of (25.5), $i = j$ or else in one of the ϵ 's two of the indices will be repeated; for the same reason in the second term $i = k$, $j = l$ or alternatively $i = l$, $j = k$. The summation over all remaining i 's gives $(n-1)!$ in the first term and $(n-2)!$ in the second; thus we obtain

$$(\Psi, H\Psi) = \sum_i \langle i | H_0(1) | i \rangle + \frac{1}{2} \sum_{i,j} \langle ij | V(1, 2) | ij \rangle_A, \quad (25.6)$$

where

$$\langle ij | V(1, 2) | ij \rangle_A = \langle ij | V(1, 2) | ij \rangle - \langle ij | V(1, 2) | ji \rangle, \quad (25.7)$$

and

$$\langle ij|V(1,2)|kl\rangle = \int \psi_i^*(1)\psi_j^*(2)V(1,2)\psi_k(1)\psi_l(2)d\tau_1d\tau_2, \quad (25.8a)$$

$$\langle i|H_0(1)|j\rangle = \int \psi_i^*(1)H_0(1)\psi_j(1)d\tau_1. \quad (25.8b)$$

The ψ_i may be expanded in terms of any convenient complete set of single-particle states $|\alpha\rangle$:

$$\psi_i = \sum_{\alpha} c_i^{\alpha} |\alpha\rangle. \quad (25.9)$$

While the expansion (25.9) in general involves an infinite number of terms, we always truncate it in approximation procedures, so that we shall assume here that (25.9) is a finite sum.

Introducing (25.9) in (25.6), we can write

$$\begin{aligned} (\Psi, H\Psi) - \sum_{i=1}^n \epsilon_i \sum_{\alpha} c_i^{\alpha*} c_i^{\alpha} &= \sum_{i=1}^n \sum_{\alpha\gamma} [c_i^{\alpha*} \langle \alpha | H_0 | \gamma \rangle c_i^{\gamma}] \\ &+ \sum_{i,j=1}^n \sum_{\substack{\alpha\beta \\ \gamma\delta}} \{c_i^{\alpha*} c_j^{\beta*} [\langle \alpha\beta | V | \gamma\delta \rangle - \langle \alpha\beta | V | \delta\gamma \rangle] c_i^{\gamma} c_j^{\delta}\} \\ &- \sum_{i=1}^n \epsilon_i \sum_{\alpha} c_i^{\alpha*} c_i^{\alpha}, \end{aligned} \quad (25.10)$$

where the ϵ_i have been introduced as Lagrange multipliers to insure normalization. A variational analysis of (25.10) implies minimizing this expression with respect to the coefficients. Taking the derivative of (25.10) with respect to $c_i^{\alpha*}$ equal to zero and remembering that c_i^{α} , and $c_i^{\alpha*}$ are independent, we arrive at the Hartree-Fock equations [2]

$$\sum_{\gamma} \langle \alpha | H_0 | \gamma \rangle c_i^{\gamma} + \sum_{\gamma} \sum_j \sum_{\beta\delta} [c_j^{\beta*} \langle \alpha\beta | V | \gamma\delta \rangle c_j^{\delta}] c_i^{\gamma} = \epsilon_i c_i^{\alpha}. \quad (25.11)$$

Eq. (25.11) is a system of cubic equations in the c_i^{α} , $c_i^{\alpha*}$. It may be solved by an iterative procedure. Let us write

$$\sum_j \sum_{\beta\delta} [c_j^{\beta*} \langle \alpha\beta | V | \gamma\delta \rangle c_j^{\delta}] \equiv \langle \alpha | U | \gamma \rangle \quad (25.12)$$

and calculate these matrix elements with initial values for the c_i^{α} , say δ_i^{α} . When we substitute the result in (25.11), we get a system of linear equations in the c_i^{α} ; this we can now solve in the standard way. If we started with

a set of K states $|\alpha\rangle$, the vectors c_i^{α} are K -dimensional and orthonormal, and so obey

$$\sum_{\alpha} c_i^{\alpha*} c_j^{\alpha} = \delta_{ij}. \quad (25.13)$$

There are thus K independent vector solutions of the linearised version of (25.11):

$$\sum_{\gamma} [\langle \alpha | H_0 | \gamma \rangle + \langle \alpha | U | \gamma \rangle] c_i^{\gamma} = \epsilon_i c_i^{\alpha}. \quad (25.14)$$

Among these solutions we select those for the n lowest eigenvalues ϵ_i and substitute them back into (25.12); this provides the starting point for the next iteration. The process is continued until self-consistency is reached, or in other words until the c_i^{α} used in (25.12) and the solutions of (25.14) obtained from them coincide to within a certain approximation.

We shall proceed to carry out in the next sections this procedure for the solution of the equations (25.11), when the configuration part of the state $|\alpha\rangle$ is a single-particle harmonic oscillator wave function. In particular we shall discuss the case of closed shells.

26 Hartree-Fock Approximation with Harmonic Oscillator States. The Case of Closed Shells

For the sake of definiteness let us assume that the Hamiltonian (25.1) corresponds to a nuclear problem [3] in which $H_0(s)$ is just the kinetic energy of the s th nucleon:

$$H_0(s) \equiv T(s), \quad (26.1)$$

while $V(s, t)$ is a central potential acting between the nucleons and including exchange terms:

$$\begin{aligned} V(s, t) &= V_W(r_{st}) + V_M(r_{st})P_{st}^M + V_B(r_{st})P_{st}^B + V_H(r_{st})P_{st}^H \\ &= V_W(r_{st}) - V_M(r_{st})(S^2 - 1)(T^2 - 1) \\ &\quad + V_B(r_{st})(S^2 - 1) - V_H(r_{st})(T^2 - 1). \end{aligned} \quad (26.2)$$

Here W, M, B, H indicate the Wigner, Majorana, Bartlett and Heisenberg interactions, while S, T are the total spin and isospin of the two particles.

We shall now take for the single-particle states $|\alpha\rangle$ of the nucleon the form

$$|\alpha\rangle = |n_\alpha l_\alpha m_\alpha\rangle |\sigma_\alpha\rangle |\tau_\alpha\rangle, \quad (26.3)$$

where $|n_\alpha l_\alpha m_\alpha\rangle$ are the harmonic oscillator states of section 1, while $|\sigma_\alpha\rangle, |\tau_\alpha\rangle$ are the usual spin and isospin wave functions.

The Hartree-Fock equations (25.11) can then be written as

$$\sum_\gamma T_{\alpha\gamma} c_i^\gamma + \sum_\gamma \sum_{j=1}^n \sum_{\beta\delta} [c_j^{\beta*} V_{\alpha\beta\gamma\delta} c_j^\delta] c_i^\gamma = \epsilon_i c_i^\alpha. \quad (26.4)$$

This involves one-body matrix elements $T_{\alpha\gamma}$ and two-body ones $V_{\alpha\beta\gamma\delta}$; the latter we already know how to expand in terms of one-body matrix elements and transformation brackets (see chapter II). Making use of the orthonormality properties of the $3j$ coefficients and the symmetry rules (10.38) for the STB , we obtain [3]

$$\begin{aligned} T_{\alpha\gamma} &\equiv \langle n_\alpha l_\alpha m_\alpha \sigma_\alpha \tau_\alpha | T(1) | n_\gamma l_\gamma m_\gamma \sigma_\gamma \tau_\gamma \rangle \\ &= \langle n_\alpha l_\alpha | T(1) | n_\gamma l_\gamma \rangle \delta_{l_\alpha l_\gamma} \delta_{m_\alpha m_\gamma} \delta_{\sigma_\alpha \sigma_\gamma} \delta_{\tau_\alpha \tau_\gamma}, \end{aligned} \quad (26.5)$$

$$\begin{aligned} V_{\alpha\beta\gamma\delta} &= \sum_{\lambda\mu} \sum_{\substack{SM_S \\ TM_T}} \sum_{\substack{NLn' \\ nl}} \left\{ (-1)^{l_\alpha+l_\beta+l_\gamma+l_\delta} (2\lambda+1)(2S+1)(2T+1) \right. \\ &\quad \times \begin{pmatrix} l_\alpha & l_\beta & \lambda \\ m_\alpha & m_\beta & -\mu \end{pmatrix} \begin{pmatrix} l_\gamma & l_\delta & \lambda \\ m_\gamma & m_\delta & -\mu \end{pmatrix} \\ &\quad \times \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S \\ \sigma_\alpha & \sigma_\beta & -M_S \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S \\ \sigma_\gamma & \sigma_\delta & -M_S \end{pmatrix} \\ &\quad \times \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \tau_\alpha & \tau_\beta & -M_T \end{pmatrix} \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T \\ \tau_\gamma & \tau_\delta & -M_T \end{pmatrix} \\ &\quad \times \langle n'l, NL, \lambda | n_\alpha l_\alpha, n_\beta l_\beta, \lambda \rangle [1 - (-1)^{l+S+T}] \\ &\quad \times \langle n'l | V_{ST}(1, 2) | nl \rangle \langle nl, NL, \lambda | n_\gamma l_\gamma, n_\delta l_\delta, \lambda \rangle \Big\}. \end{aligned} \quad (26.6)$$

Eq. (26.2) allows us to write explicitly the two-body potential in (26.6):

$$\begin{aligned} V_{ST}(1, 2) &= V_W(r_{12}) - V_M(r_{12})[S(S+1)-1][T(T+1)-1] \\ &\quad + V_B(r_{12})[S(S+1)-1] - V_H(r_{12})[T(T+1)-1]. \end{aligned} \quad (26.7)$$

In (26.7), the factors $V_W(r_{12})$ and so on give the radial dependence of the components in (26.2). The methods of section 2 then give us the reduced matrix elements of $T(1)$ and $V_{ST}(1, 2)$.

Finally, let us indicate explicitly on what quantum numbers depend the coefficients c_i^α by writing

$$c_i^\alpha \equiv c_i^{n_\alpha l_\alpha m_\alpha \sigma_\alpha \tau_\alpha}. \quad (26.8)$$

Thus everything in (26.4) is completely defined, and we can solve this equation systematically, as outlined in the previous section.

A case of some interest is that of the n particles occupying orbits in a central potential whose parameters are to be found from the Hartree-Fock analysis. This implies that the index i of the states in which we find the particles can be decomposed into

$$i = \nu_i l_i m_i \sigma_i \tau_i, \quad (26.9)$$

where $l_i, m_i, \sigma_i, \tau_i$ are respectively the orbital angular momentum and its projection, and the projection of spin and isospin that characterize the state. The index ν_i characterizes the radial states in this, as yet, undetermined central potential. Clearly the coefficient c_i^α can now be written as

$$c_i^\alpha = c_{\nu_i}^{n_\alpha} (l_\alpha m_\alpha \sigma_\alpha \tau_\alpha) \delta_{l_i}^{l_\alpha} \delta_{m_i}^{m_\alpha} \delta_{\sigma_i}^{\sigma_\alpha} \delta_{\tau_i}^{\tau_\alpha}. \quad (26.10)$$

We shall now assume that the particles fill all orbits in this central potential up to a given level; then for each filled ν_i, l_i , we have particles in states with all values $m_i = l_i, l_i - 1, \dots, -l_i$, $\sigma_i = +\frac{1}{2}, -\frac{1}{2}$, $\tau_i = +\frac{1}{2}, -\frac{1}{2}$. We proceed to show that in this case $c_{\nu_i}^{n_\alpha}$ depends only on l_α , that is, that we can write

$$c_i^\alpha = c_{\nu_i}^{n_\alpha} (l_\alpha) \delta_{l_i}^{l_\alpha} \delta_{m_i}^{m_\alpha} \delta_{\sigma_i}^{\sigma_\alpha} \delta_{\tau_i}^{\tau_\alpha}. \quad (26.11)$$

It is enough for this purpose to prove that, if we introduce (26.11) into (26.4), the resulting equations will be independent of the indices m, σ and τ .

We start by realizing that (26.11) implies

$$\sum_j c_j^{\beta*} c_j^\delta = \sum_{\nu_j} c_{\nu_j}^{n_\beta} (l_\beta) c_{\nu_j}^{n_\delta} (l_\beta) \delta_{l_\beta l_\delta} \delta_{m_\beta m_\delta} \delta_{\sigma_\beta \sigma_\delta} \delta_{\tau_\beta \tau_\delta}. \quad (26.12)$$

Introducing this expression into the square bracket in (26.4) and remembering that we have to carry out summations over all $m_\beta = l_\beta, l_\beta - 1, \dots, -l_\beta$, $\sigma_\beta = \pm\frac{1}{2}$, $\tau_\beta = \pm\frac{1}{2}$, we obtain

$$\begin{aligned} \sum_j \sum_{\beta\delta} [c_j^{\beta*} V_{\alpha\beta\gamma\delta} c_j^\delta] &= \sum_{\nu_j} \sum_{n_\beta n_\delta} \sum_{l_\beta} \\ &\times \left[c_{\nu_j}^{n_\beta*}(l_\beta) \sum_{\lambda ST} \sum_{\substack{n'nl \\ NL}} \left\{ \frac{(2\lambda+1)(2S+1)(2T+1)}{4(2l_\alpha+1)} \right. \right. \\ &\times \langle n'l, NL, \lambda | n_\alpha l_\alpha, n_\beta l_\beta, \lambda \rangle [1 - (-1)^{l+S+T}] \langle n'l | V_{ST}(1, 2) | nl \rangle \\ &\times \langle nl, NL, \lambda | n_\gamma l_\alpha, n_\delta l_\beta, \lambda \rangle \left. \left. \right\} c_{\nu_j}^{n_\delta}(l_\beta) \right] \delta_{l_\alpha l_\gamma} \delta_{m_\alpha m_\gamma} \delta_{\sigma_\alpha \sigma_\gamma} \delta_{\tau_\alpha \tau_\gamma}, \quad (26.13) \end{aligned}$$

where we made use of the relation

$$\begin{aligned} \sum_{m_\beta m_\delta \mu} (-1)^{l_\alpha + l_\beta + l_\gamma + l_\delta} (2\lambda + 1) &\left(\begin{array}{ccc} l_\alpha & l_\beta & \lambda \\ m_\alpha & m_\beta & -\mu \end{array} \right) \\ &\times \left(\begin{array}{ccc} l_\gamma & l_\delta & \lambda \\ m_\gamma & m_\delta & -\mu \end{array} \right) \delta_{m_\beta m_\delta} \delta_{l_\beta l_\delta} \\ &= \frac{2\lambda + 1}{2l_\alpha + 1} \sum_{m_\beta \mu} (-1)^{l_\alpha + l_\gamma} (2l_\alpha + 1) \\ &\times \left(\begin{array}{ccc} l_\beta & \lambda & l_\alpha \\ m_\beta & -\mu & m_\alpha \end{array} \right) \left(\begin{array}{ccc} l_\beta & \lambda & l_\gamma \\ m_\beta & -\mu & m_\gamma \end{array} \right) \\ &= \frac{2\lambda + 1}{2l_\alpha + 1} \delta_{l_\alpha l_\gamma} \delta_{m_\alpha m_\gamma}, \quad (26.14) \end{aligned}$$

and similar ones for the spin and isospin $3j$ coefficients.

Substituting (26.13) into (26.4) and eliminating the common multiplicative factor $\delta_{l_i}^{l_\alpha} \delta_{m_i}^{m_\alpha} \delta_{\sigma_i}^{\sigma_\alpha} \delta_{\tau_i}^{\tau_\alpha}$ we obtain for the coefficients $c_{\nu_i}^{n_\alpha}(l_\alpha)$ the set of equations

$$\begin{aligned} \sum_{n_\gamma} \langle n_\alpha l_\alpha | T | n_\gamma l_\alpha \rangle c_{\nu_i}^{n_\gamma}(l_\alpha) &+ \sum_{n_\gamma} \sum_{\nu_j} \sum_{n_\beta n_\delta} \sum_{l_\beta} \left[c_{\nu_j}^{n_\beta*}(l_\beta) \sum_{\lambda ST} \sum_{\substack{n'nl \\ NL}} \left\{ \frac{(2\lambda+1)(2S+1)(2T+1)}{4(2l_\alpha+1)} \right. \right. \\ &\times \langle n'l, NL, \lambda | n_\alpha l_\alpha, n_\beta l_\beta, \lambda \rangle [1 - (-1)^{l+S+T}] \\ &\times \langle nl, NL, \lambda | n_\gamma l_\alpha, n_\delta l_\beta, \lambda \rangle \langle n'l | V_{ST}(1, 2) | nl \rangle \left. \left. \right\} c_{\nu_j}^{n_\delta}(l_\beta) \right] c_{\nu_i}^{n_\gamma}(l_\alpha) \\ &= \epsilon_i c_{\nu_i}^{n_\alpha}(l_\alpha). \quad (26.15) \end{aligned}$$

We have proved, then, that for closed shells we can assume the form (26.11) for the coefficients c_i^α in (26.4); these equations then transform

into (26.15). This means considerable reduction and simplification in the equations and the work of solving them, because in (26.15) all dependence on the indices m, σ, τ has disappeared.

We have obtained the Hartree-Fock equations for one of the forces in the nuclear case. When dealing with atoms, there are several differences to notice. Firstly, instead of just the kinetic-energy term, we have for the single-body part of the Hamiltonian (in the units of section 3)

$$H_0 = \frac{1}{2}\epsilon^2 p^2 - \frac{Z\epsilon\sqrt{2}}{r}. \quad (26.16)$$

Secondly, the isotopic spin τ does not appear in the description of the states; this eliminates the index T in $V_{ST}(1, 2)$, a factor $(-1)^{T-1}$ appearing in $[1 - (-1)^{l+S+T}]$ and a factor $\frac{1}{2}(2T+1)$, all in (26.15) and the equations leading up to it. Finally, the Coulomb force is of Wigner type, and therefore $V_S(1, 2)$ is independent of S . Hence we can sum over S in the corresponding factors of (26.15); we get

$$\sum_S \frac{1}{2}(2S+1)[1 + (-1)^{l+S}] = 2 - (-1)^l. \quad (26.17)$$

Thus, from (26.15), we can straightforwardly get the corresponding set of Hartree-Fock equations in the atomic case.

Had we decided to use for the single-particle states $|\alpha\rangle$, the form in which spin and orbital angular momentum are coupled to j ,

$$|\alpha\rangle = |n_\alpha l_\alpha j_\alpha m_\alpha\rangle |\tau_\alpha\rangle, \quad (26.18)$$

the analysis could have been carried out in a very similar way, with the main difference that in the reduction of the two-body to the one-body matrix elements we would have to use the procedure in $j-j$ coupling developed in section 13. Again, when dealing with closed shells, for which all values $\tau_i = \pm\frac{1}{2}$, $m_i = j_i, j_i - 1, \dots, -j_i$; are occupied, we see that the Hartree-Fock equations become independent of m, τ .

In the next section we apply the analysis developed here for closed shells to some atomic and nuclear problems.

27 Application to the Beryllium Atom and the ^{16}O Nucleus

The beryllium atom is a closed-shell system of four electrons which in the usual spectroscopic notation is characterized by the configuration [4]

$(1s)^2(2s)^2$ 1S_0 . This implies that the single-particle states in the Hartree-Fock approximation are all of orbital angular momentum and projection zero. This still leaves the possibilities $\sigma = \pm \frac{1}{2}$ for the projection of the spin of the electrons; but since there are four spins to accommodate, we must put two in a radial state — call it $\nu = 1$ — and the other two in a second radial state $\nu = 2$. Hence we see that the Hartree-Fock equations (26.15), particularized to the atomic case, will take the following form for the beryllium atom, whose configuration has $l_\alpha = l_\beta = 0$:

$$\begin{aligned} & \sum_{n_1} \langle n'_1 0 | \frac{1}{2} \epsilon^2 (\mathbf{p}_1)^2 - \frac{\sqrt{2}\epsilon}{|\mathbf{x}_1|} \| n_1 0 \rangle c_\nu^{n_1} \\ & + \sum_{n_1} \sum_{\nu'} \sum_{n'_2 n_2} \left[c_\nu^{n'_2 *} \sum_{n' n N} \left\{ (2\lambda + 1) \langle n' l, NL, 0 | n'_1 0, n'_2 0, 0 \right. \right. \\ & \times [2 - (-1)^l] \langle n' l | \frac{\epsilon}{|\mathbf{x}_1|} \| n l \rangle \langle n l, NL, 0 | n_1 0, n_2 0, 0 \left. \right\} c_\nu^{n_2} \right] c_\nu^{n_1} \\ & \equiv \epsilon_\nu c_\nu^{n'_1}. \end{aligned} \quad (27.1)$$

By $\mathbf{p}_1, \mathbf{x}_1, \dot{\mathbf{x}}_1 = (1/\sqrt{2})(\mathbf{x}_1 - \mathbf{x}_2)$, we denote the dimensionless coordinates and momenta as defined in (3.2). In (27.1) we made the following changes in notation as compared with (26.15):

$$n_\alpha = n'_1, n_\beta = n'_2, n_\gamma = n_1, n_\delta = n_2, \nu_j = \nu', \nu_i = \nu, \quad (27.2)$$

where ν and ν' take only the values 1 and 2, and we write $c_\nu^n(l=0) \equiv c_\nu^n$.

The number of equations in (27.1) is equal to the number of harmonic oscillator states we consider in the expansion

$$\psi_\nu = \sum_n c_\nu^n |n00\rangle, n = 0, 1, \dots, \frac{1}{2}\mathfrak{N}, \quad (27.3)$$

that is, $1+\mathfrak{N}/2$ where \mathfrak{N} is the maximum number of quanta in the expansion and, because of the parity of the states with $l=0$, \mathfrak{N} is restricted to even values.

The equations (27.1) may be solved by the recursion procedure discussed in §25; this gives the coefficients c_ν^n in (27.3) and so allows us in turn to calculate the expectation value of the energy for the four-electron antisymmetric state given by (25.6).

This programme was implemented by Calles and Dubovoy [5] for the Be atom. They started by assuming the following form for the single-particle states:

$$\psi_1 = |000\rangle, \quad \psi_2 = |100\rangle, \quad (27.4)$$

for which the expectation value of the energy (25.6) becomes

$$\langle \Psi, H\Psi \rangle = 5\epsilon^2 - 18.2149\epsilon, \quad (27.5)$$

with, as indicated in (3.3), $\epsilon = [\hbar\omega/(me^4/2\hbar^2)]^{\frac{1}{2}}$. Minimizing this energy with respect to ϵ we get

$$\epsilon = 1.82, \quad (27.6a)$$

$$\langle H \rangle = -16.59. \quad (27.6b)$$

Note that all the energies in the atomic problems discussed here are given in units of

$$\frac{me^4}{2\hbar^2} = 13.6 \text{ eV}. \quad (27.7)$$

For the next step Calles and Dubovoy [5] consider the expansion

$$\psi_\nu = c_\nu^0 |000\rangle + c_\nu^1 |100\rangle + c_\nu^2 |200\rangle + c_\nu^3 |300\rangle \quad (27.8)$$

and show that a self-consistent solution of the equations (27.1), in which they take for ϵ the value (27.6a), is achieved after four steps. The values of the coefficients c_ν^n and the corresponding ϵ 's they obtain are

$$\begin{aligned} \epsilon_1 &= -6.42, \quad c_1^0 = 0.886, \quad c_1^1 = 0.359, \quad c_1^2 = 0.219, \quad c_1^3 = 0.194, \\ \epsilon_2 &= 0.10, \quad c_2^0 = -0.316, \quad c_2^1 = 0.833, \quad c_2^2 = -0.345, \quad c_2^3 = 0.295. \end{aligned} \quad (27.9)$$

From these values of c_ν^n we in turn get for the expectation value of the energy the value

$$\langle H \rangle = -21.37. \quad (27.10)$$

The experimental energy of the ground state of the Be atom is, in the units (27.7), -28.74 . Thus we get 74% of the binding energy in the approximation (27.8). Since a computer programme for solving the set of equations (27.1) with \mathfrak{N} large is easy to write, and since programmes for the transformation brackets and coefficients $B(n'l', nl, p)$ are available, much more extensive calculations for the Be atom can be carried out.

Let us now turn to the application of Hartree-Fock calculations with harmonic oscillator states in the field of nuclear physics. Important contributions in this field are due to Davies, Krieger and Baranger [3] (DKB);

they have carried out extensive calculations for many nuclei in the periodic table. We shall discuss here only their results for the closed shell nucleus ^{16}O .

The first thing needed for the solution of the equations (26.15) in the nuclear case, is the knowledge of the two-particle interaction $V_{ST}(1, 2)$. Clearly it is not possible to consider interactions with hard cores, since the integration for the matrix element $\langle n'l' | V_{ST}(1, 2) | nl \rangle$ will blow up. Instead DKB propose a velocity-dependent interaction which acts only between states of relative angular momentum $l = 0$, so that

$$\langle n'l' | V_{ST}(1, 2) | nl \rangle = \delta_{l0} \langle n'0 | V_{ST}(1, 2) | nl \rangle. \quad (27.11)$$

Because of the factor $[1 - (-1)^{l+S+T}]$ in (26.15) we see that if $l = 0$ we are restricted to either $S = 0, T = 1$ or $S = 1, T = 0$. The velocity-dependent interaction potential that DKB propose is

$$V_{ST} = \frac{\hbar^2}{m} [U_S(r') + p'^2 W_S(r') + W_S(r') p'^2], \quad (27.12a)$$

where

$$U_S(r') = -A_S \exp(-\alpha_S^2 r'^2), \quad (27.12b)$$

$$W_S(r') = B_S \exp(-\alpha_S^2 r'^2), \quad (27.12c)$$

$$T = \frac{1}{2}[1 + (-1)^S], \quad (27.12d)$$

and (as in section 5) r', p' are the magnitudes of coordinates and momenta in ordinary units.

The values of A_S, B_S, α_S that DKB assume are the following:

S	$A_S(\text{fm}^{-2})$	B_S	$\alpha_S(\text{fm}^{-1})$	
0	0.835	0.60	0.50	
1	2.56	0.50	0.70	

(27.12e)

The potential (27.12), acting only between $l = 0$ states, was chosen mainly to give a good fit to the binding energy of nuclear matter. Its fit to the two-body scattering data is rather poor.

Using (27.11) and the notation (27.2), the Hartree-Fock equations (26.15) for closed shells take now the following form [3]:

Table V.1. Expectation values of the total energy $\langle H \rangle$ and the single-particle energies $\epsilon_1(l)$, both in MeV. The coefficients $c_1^n(l)$ for the expansion of the single-particle states in terms of harmonic-oscillator states are also given. All of these magnitudes are functions of the dimensionality d of the system of linear equations that determines them.

d	$\langle H \rangle$	1s state						1p state										
		$c_1^0(0)$	$c_1^1(0)$	$c_1^2(0)$	$c_1^3(0)$	$c_1^4(0)$	$c_1^5(0)$	$c_1^6(0)$	$c_1^7(0)$	$c_1^0(1)$	$c_1^1(1)$	$c_1^2(1)$	$c_1^3(1)$	$c_1^4(1)$	$c_1^5(1)$	$c_1^6(1)$	$c_1^7(1)$	
3	-78.289	-40.592	-16.173	0.98425	0.17255	0.03836				0.99363	0.09967	0.05257						
4	-78.298	-40.610	-16.173	0.98414	0.17329	0.03752	0.00552			0.99361	0.09963	0.05303	-0.00094					
5	-78.301	-40.611	-16.171	0.98413	0.17335	0.03763	0.00535	0.00083		0.99360	0.09950	0.05342	-0.00177	0.00195				
6	-78.303	-40.610	-16.170	0.98413	0.17334	0.03762	0.00537	0.00072	0.00035	0.99359	0.09944	0.05355	-0.00209	0.00265	-0.00145			
7	-78.303	-40.609	-16.170	0.98413	0.17333	0.03762	0.00536	0.00077	0.00018	0.00051	0.99359	0.09943	0.05357	-0.00214	0.00277	-0.00169	0.00047	
8	-78.303	-40.609	-16.170	0.98413	0.17333	0.03762	0.00536	0.00075	0.00023	0.00033	0.00048	0.99359	0.09943	0.05357	-0.00214	0.00277	-0.00169	0.00046

$$\begin{aligned} & \sum_{n_1} \langle n'_1 l_1 \| \frac{1}{2m} p'^2 \| n_1 l_1 \rangle c_\nu^{n_1}(l_1) \\ & + \sum_{n_1} \sum_{\nu'} \sum_{n'_2 n_2} \sum_{l_2} \left\{ c_{\nu'}^{n'_2*}(l_2) \sum_{\substack{n' n \\ l N}} \left(\frac{3}{2} \frac{2\lambda + 1}{2l_1 + 1} \right) \right. \\ & \times \langle n' 0, N\lambda, \lambda | n'_1 l_1, n'_2 l'_2, \lambda | [\langle n' 0 \| V_{01} \| n 0 \rangle + \langle n' 0 \| V_{10} \| n 0 \rangle] \\ & \left. \times \langle n 0, N\lambda, \lambda | n_1 l_1, n_2 l_2, \lambda | c_{\nu'}^{n_2}(l_2) \right\} c_\nu^{n_1}(l_1) = \epsilon_\nu(l_1) c_\nu^{n'_1}(l_1); \quad (27.13) \end{aligned}$$

and from (3.10) we have

$$\begin{aligned} \langle n'_1 l_1 \| \frac{1}{2m} p'^2 \| n_1 l_1 \rangle &= \frac{1}{2} \hbar \omega \left[(n_1(n_1 + l_1 + \frac{1}{2}))^{\frac{1}{2}} \delta_{n'_1 n_1 + 1} \right. \\ &+ (2n_1 + l_1 + \frac{3}{2}) \delta_{n'_1 n_1} + ((n_1 + 1)(n_1 + l_1 + \frac{3}{2}))^{\frac{1}{2}} \delta_{n'_1 n_1 - 1} \left. \right]. \quad (27.14) \end{aligned}$$

The matrix element of V_{ST} , besides terms $\langle n' 0 \| U \| n 0 \rangle$, has also terms of the type

$$\langle n' 0 \| p'^2 W(r') \| n 0 \rangle = \sum_{n''} \langle n' 0 \| p'^2 \| n'' 0 \rangle \langle n'' 0 \| W(r') \| n 0 \rangle, \quad (27.15)$$

where the first factor in the summation is given in (27.14), while the second can be obtained in the usual way discussed in section 2.

The calculations for ^{16}O by DKB were done with

$$\left(\frac{\hbar}{m\omega} \right)^{1/2} = 2.1 \text{ fm.} \quad (27.16)$$

In this nucleus, we have four nucleons in the states for which $l_1 = 0$ and twelve in the $l_1 = 1$ states. We have then two separate problems in (27.13) for $l_1 = 0$ and $l_1 = 1$ though in the square bracket the summation over l_2 must be over both values. The dimensionality d for the system of linear equations will be the number of different n 's we take. Thus if we take $n = 0, 1, 2$ then $d = 3$; for $n = 0, 1, 2, 3$ it is $d = 4$, etc. The approximation should become better as d increases. The eigenvalues $\epsilon_\nu(l)$ give the energy levels in the equivalent one-body potential. In particular we are interested in $\nu = 1$ when $l = 0, 1$, i.e., the energies of the $1s$ and $1p$ states. Furthermore once we solve the equations (27.13) self consistently we get the coefficients $c_1^n(l)$ corresponding to the eigenvalues $\epsilon_1(l)$. With these coefficients we can calculate the expectation value $\langle H \rangle$ of the energy

given by (25.6). In Table V.1 we give DKB's results for $\epsilon_1(l)$, $c_1^n(l)$ and $\langle H \rangle$ for the dimensionalities 3, 4, 5, 6, 7 and 8.

The examples presented here illustrated the application of harmonic oscillator states to Hartree-Fock calculations in atomic and nuclear problems. We refer the reader to the original literature for much more extensive applications [3,6].

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Chapter VI

The Harmonic Oscillator in Scattering and Reaction Theory

In previous chapters we discussed the application of harmonic oscillator basis in the description of bound states of atoms, molecules and nuclei. This basis can also be used for description of states in the continuum as happens in scattering and reaction problems [1–6].

28 Scattering of a Particle in a Central Potential

In order to illustrate the essence of our problem we shall consider first the one of a particle scattered by a central short range (*i.e.*, going to 0 faster than r^{-1} if $r \rightarrow \infty$) potential. Using, as before, units in which

$$\hbar = m = \omega = 1, \quad (28.1)$$

where ω is the frequency of the oscillator potential we employ in the following calculations, our Schroedinger equation can be written as

$$\left[\frac{1}{2} p^2 + V(r) \right] \psi_{lm}(r) = E \psi_{lm}(r), \quad (28.2)$$

because the orbital angular momentum L^2 , and its projection L_z are integrals of motion, so ψ can be characterized by their eigenvalues l, m .

Furthermore the momentum p , the coordinate r and energy E are given in the dimensionless units of Eq. (3.2).

The solution of (28.2) has the form

$$\psi_{lm}(r) = R_l(r)Y_{lm}(\theta, \phi), \quad (28.3)$$

where in turn the $R_l(r)$ will be sought in a form of an expansion in terms of radial harmonic oscillator functions, *i.e.*,

$$R_l(r) = \sum_{n'=0}^{\infty} (-1)^{n'} C_{n'l} R_{n'l}(r), \quad (28.4)$$

where $R_{n'l}(r)$ is given by (1.8), but here we shall also write them in terms of Laguerre polynomials in the well known form [7]

$$R_{nl}(r) = \left[\frac{2(n!)}{\Gamma(n+l+\frac{3}{2})} \right]^{1/2} r^l L_n^{l+\frac{1}{2}}(r^2) e^{-\frac{1}{2}r^2}. \quad (28.5)$$

It is clear from Eq. (28.4) that

$$C_{nl} \equiv (-1)^n \langle R_{nl}(r) | R_l(r) \rangle = (-1)^n \int_0^\infty r^2 dr R_{nl}(r) R_l(r). \quad (28.6)$$

A phase factor $(-1)^n$ is introduced in (28.4) to correlate the notation followed in the previous chapters, with that of references [3,4,6], as well as for later convenience.

The radial function (28.5) corresponds to the energy $E_{nl} = (2n+l+\frac{3}{2})$ in the present units and, in ordinary units, it would have to be multiplied by $\hbar\omega$. On the other hand, the energy E appearing in problem (28.2) can be expressed in terms of a wave number k as $E = (k^2/2)$ where k could be transformed to ordinary units using (3.2).

Substituting expansion (28.4) in (28.2), multiplying the latter by $(-1)^{-n} \times R_{nl}(r) Y_{lm}^*$, and integrating over the configuration space we get the equations

$$\sum_{n'} (H_{nn'} - \delta_{nn'} E) (-1)^{n'-n} C_{n'l} = 0, \quad n = 0, 1, 2, \dots, \quad (28.7)$$

which become

$$\begin{aligned} & - [n(n+l+\frac{1}{2})]^{1/2} C_{n-1l} + (2n+l+\frac{3}{2}) C_{nl} \\ & - [(n+1)(n+l+\frac{3}{2})]^{1/2} C_{n+1l} + 2 \sum_{n'} (-1)^{n'-n} \\ & \times \langle nl | V | n'l \rangle C_{n'l} = k^2 C_{nl}, \end{aligned} \quad (28.8)$$

where we used the relation (28.6) and the fact that for the kinetic energy $T = p^2/2$ the only non vanishing matrix elements are

$$T_{nn-1}^l = \frac{1}{2} [n(n+l+\frac{1}{2})]^{1/2} \quad (28.9a)$$

$$T_{nn}^l = \frac{1}{2} [2n+l+\frac{3}{2}] \quad (28.9b)$$

$$T_{nn+1}^l = \frac{1}{2} [(n+1)(n+l+\frac{3}{2})]^{1/2}, \quad (28.9c)$$

as shown in (3.10).

For a short range potential the matrix element $\langle nl | V | n'l \rangle$ diminishes quickly as $n, n' \rightarrow \infty$ as the wave function $R_{nl}(r)$ oscillates very rapidly when n, n' are large. Thus the effect of the potential matrix element can be cut at some appropriate maximum value N of n, n' and Eq. (28.8) can be broken into three sets:

$$\begin{aligned} & \sum_{n'=0}^N (-1)^{n'-n} (H_{nn'} - E \delta_{nn'}) C_{n'l} \\ & = \delta_{nN} T_{NN+1}^l C_{N+1l}, \quad n \leq N \end{aligned} \quad (28.10a)$$

$$\begin{aligned} & -T_{N+1N}^l C_{Nl} + (T_{N+1N+1}^l - E) C_{N+1l} \\ & - T_{N+1N+2}^l C_{N+2l} = 0, \end{aligned} \quad (28.10b)$$

$$\begin{aligned} & -T_{nn-1}^l C_{n-1l} + (T_{nn}^l - E) C_{nl} \\ & - T_{nn+1}^l C_{n+1l} = 0, \quad n \geq N+1. \end{aligned} \quad (28.10c)$$

Thus the coefficients C_{nl} with $n > N$ obey the recurrence relation for free motion (28.10c), and the first step in the solution of Eq. (28.10) consists in finding two linear independent functions that satisfy (28.10c), *i.e.*, that correspond to free motion for which the solution of Eq. (28.2) can be immediately written. The next step will be to connect the external with the internal part, satisfying respectively (28.10c) and (28.10a) through the intermediate equation (28.10b).

The solution of the scattering problem with the help of harmonic oscillator basis is then similar to the procedure followed in configuration space, where one first solved (28.2) outside and inside the range of the potential and connects them at the point where the potential ends.

We also note that the procedure indicated in Eqs. (28.10) corresponds to the exact solution of a problem of Hamiltonian $H = T + V^N$ where V^N is a separable potential of the form

$$V^N = \sum_{n,n'}^N \langle nl | V | n'l \rangle | nl \rangle \langle n'l |. \quad (28.11)$$

The nonlocal operator $| nl \rangle \langle n'l |$ acts on the wave function $R_l(r)$ as follows:

$$|nl\rangle\langle n'l|R_l(r) \equiv R_{nl}(r) \int_0^\infty r'^2 dr' R_{n'l}(r') R_l(r'). \quad (28.12)$$

29 Solution of the Equation for Free Motion in the Harmonic Oscillator Basis

Equation (28.2) when there is no potential, i.e., $V = 0$ and $E = k^2/2$ has solutions, in terms of spherical coordinates, given by $Y_{lm}(\theta, \phi)$ multiplied by either

$$j_l(kr) \text{ going into } (kr)^{-1} \sin(kr - l\frac{\pi}{2}) \text{ if } r \rightarrow \infty, \quad (29.1)$$

which is the regular solution, or

$$\begin{aligned} n_l(kr) \equiv (-1)^{l+1} j_{-l-1}(kr) &\text{ going into} \\ &-(kr)^{-1} \cos(kr - l\frac{\pi}{2}) \text{ if } r \rightarrow \infty, \end{aligned} \quad (29.2)$$

which is one of the forms of the irregular solutions [8].

The two types of functions should appear from the solutions of the set of equations (28.10c) when we assume them valid in the whole range of integer n, n' from 0 to ∞ .

To find the explicit form of the coefficients C_{nl} corresponding regular free particle problem it is then sufficient to substitute the function $\sqrt{2/\pi} j_l(kr)$ to Eq. (28.6):

$$C_{nl}^{\text{reg}}(k) = (-1)^n \sqrt{\frac{2}{\pi}} \int_0^\infty r^2 dr R_{nl}(r) j_l(kr). \quad (29.3)$$

This integral can be found in a table of definite integrals [9], but we shall proceed here in a more physical way.

We recall that the expansion of plane wave in term of spherical ones is given by [10]

$$\exp(i\mathbf{kr}) = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^*(\hat{\mathbf{k}}), \quad (29.4a)$$

where $\hat{\mathbf{r}}, \hat{\mathbf{k}}$ are the unit vectors in the direction of \mathbf{r}, \mathbf{k} respectively. If we take the scalar product of the momentum eigenvector

$$|\mathbf{k}\rangle = (2\pi)^{-3/2} \exp(i\mathbf{kr}), \quad (29.4b)$$

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with an harmonic oscillator wave function in spherical coordinates, which we indicate by the bra $\langle nlm|$, we get the same harmonic oscillator function in terms of \mathbf{k} but with an extra phase

$$\langle nlm|\mathbf{k}\rangle = i^l (-1)^n R_{nl}(k) Y_{lm}^*(\hat{\mathbf{k}}). \quad (29.5a)$$

On the other hand from (29.4) we see that

$$\langle nlm|\mathbf{k}\rangle = i^l \sqrt{\frac{2}{\pi}} \left[\int_0^\infty R_{nl}(r) j_l(kr) r^2 dr \right] Y_{lm}^*(\hat{\mathbf{k}}). \quad (29.5b)$$

Thus

$$\sqrt{\frac{2}{\pi}} \left[\int_0^\infty R_{nl}(r) j_l(kr) r^2 dr \right] = (-1)^n R_{nl}(k). \quad (29.5c)$$

Therefore the coefficients $C_{nl}(k)$ belonging to the regular solution become

$$\begin{aligned} C_{nl}^{\text{reg}}(k) = R_{nl}(k) &= \left[\frac{2(n!)^2}{\Gamma(n+l+3/2)} \right]^{1/2} k^l L_n^{l+1/2}(k^2) e^{-k^2/2} \\ &= \left[\frac{2\Gamma(n+l+3/2)}{\Gamma(n+1)} \right]^{1/2} \frac{k^l e^{-k^2/2}}{\Gamma(l+\frac{3}{2})} M(-n, l+3/2; k^2), \end{aligned} \quad (29.6)$$

where we made use of (28.5) and wrote the r.h.s. in term of the confluent hypergeometric function, $M(a, c; z)$ [7], as this will prove useful when we pass to the discussion of the irregular solution of Eq. (28.10c).

Using the asymptotic expression for the Laguerre polynomial [7] at $n \gg 1$ we obtain

$$R_{nl}(k) \sim \frac{2^{3/2}}{\pi^{1/2}} n^{1/4} j_l(2\sqrt{n}k). \quad (29.7)$$

This result will be required later.

We now turn our attention to the irregular solution of Eq. (28.10c). For this purpose we note that $T_{n'n}^l$ of (28.9) remain invariant if we make the replacement

$$n \rightarrow n + l + 1/2, \quad (29.8a)$$

$$l \rightarrow -l - 1, \quad (29.8b)$$

and therefore Eq. (28.10c) remains invariant under this substitution, so a new, and independent, solution of this equation can be obtained if in (29.6) we make in the replacement (29.8), i.e.,

$$\begin{aligned} C_{nl}^{\text{irreg}}(k) &= (-1)^{l+1} \left[\frac{2\Gamma(n+1)}{\Gamma(n+l+3/2)} \right]^{1/2} \\ &\times \frac{1}{\Gamma(-l+1/2)} k^{-l-1} e^{-k^2/2} M(-n - l - 1/2, -l + 1/2; k^2) \\ &\simeq \frac{2^{3/2}}{\pi^{1/2}} n^{1/4} n_l(2\sqrt{n}k), \end{aligned} \quad (29.9)$$

where the asymptotic behaviour of $C_{nl}^{\text{irreg}}(k)$ when $n \gg 1$ is given at the right hand side and is obtained from (29.7) if we replace in it l by $-l-1$. The additional factor $(-1)^{l+1}$ is introduced into the expression (29.9) so that the asymptotic form of $C_{nl}^{\text{irreg}}(k)$ corresponds to the solution of the free particle problem of the Neumann type (29.2).

We now proceed to show that for the difference equation (28.10c) there is property analogous to that of the Wronskian in ordinary differential equations.

If we have two solutions of Eq. (28.10c) that we denote by C_{nl} , \bar{C}_{nl} , suppressing the value k of the wave numbers, they satisfy the equations ($T_{n+1n}^l = T_{n+1n}^l$)

$$-T_{n+1n}^l C_{n+1l} + (T_{nn}^l - E) C_{nl} - T_{nn-1}^l C_{n-1l} = 0, \quad (29.10a)$$

$$-T_{n+1n}^l \bar{C}_{n+1l} + (T_{nn}^l - E) \bar{C}_{nl} - T_{nn-1}^l \bar{C}_{n-1l} = 0. \quad (29.10b)$$

Multiplying (29.10a) by \bar{C}_{nl} and (29.10b) by C_{nl} and subtracting we get the relation

$$\begin{aligned} & T_{n+1n}^l [C_{n+1l} \bar{C}_{nl} - C_{nl} \bar{C}_{n+1l}] \\ &= T_{nn-1}^l [C_{nl} \bar{C}_{n-1l} - C_{n-1l} \bar{C}_{nl}], \end{aligned} \quad (29.11)$$

which means that the combination on the left or the right hand side is independent of n and we can thus write

$$T_{n+1n}^l (C_{n+1l} \bar{C}_{nl} - C_{nl} \bar{C}_{n+1l}) \equiv K(C, \bar{C}), \quad (29.12)$$

where clearly K depends on the nature of the two solutions of the problem but not on the index n . If \bar{C}_n is a multiple of C_n , i.e., if they are linearly dependent, $K = 0$; if $K \neq 0$ we expect that implies linear independence of the two solutions just as in the case of the Wronskian.

For the particular case when \bar{C}_n , C_n refer to the regular and irregular solutions of (28.10c) given respectively by (29.6) and (29.9), we can use their asymptotic forms when $n \gg 1$ to find out that

$$K = T_{n+1n}^l [C_{nl}^{\text{reg}}(k) C_{n+1l}^{\text{irreg}}(k) - C_{nl}^{\text{irreg}}(k) C_{n+1l}^{\text{reg}}(k)] = \frac{1}{\pi k}. \quad (29.13)$$

In fact, using the asymptotic expressions for the Bessel and Neumann functions we obtain for large n

$$C_{nl}^{\text{reg}}(k) \simeq \frac{\sqrt{2}}{\sqrt{\pi} n^{1/4} k} \sin \left(2\sqrt{n}k - \frac{l\pi}{2} \right), \quad (29.14)$$

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$$C_{nl}^{\text{irreg}}(k) \simeq -\frac{\sqrt{2}}{\sqrt{\pi} n^{1/4} k} \cos \left(2\sqrt{n}k - \frac{l\pi}{2} \right). \quad (29.15)$$

Then the expression (29.13) can be calculated as follows:

$$\begin{aligned} K &= T_{n+1n}^l \det \begin{vmatrix} C_{nl}^{\text{reg}}(k) & C_{n+1l}^{\text{reg}}(k) \\ C_{nl}^{\text{irreg}}(k) & C_{n+1l}^{\text{irreg}}(k) \end{vmatrix} \\ &\simeq \frac{n}{2} \det \begin{vmatrix} C_{nl}^{\text{reg}}(k) & \partial C_{nl}^{\text{reg}}(k)/\partial n \\ C_{nl}^{\text{irreg}}(k) & \partial C_{nl}^{\text{irreg}}(k)/\partial n \end{vmatrix}. \end{aligned} \quad (29.16)$$

Substituting here the asymptotic forms (29.7) and (29.9) we obtain the result (29.13). Here be used the equalities

$$T_{n+1n}^l \simeq \frac{1}{2} n, \quad C_{n+1l} \simeq C_{nl} + \frac{\partial}{\partial n} C_{nl} \quad (29.17)$$

that are valid at $n \gg 1$.

30 Calculation of Phase Shifts

It is known that in the asymptotic region $r \rightarrow \infty$ where the potential $V(r) \rightarrow 0$ the coordinate wave function for the scattering states is a linear combination of the regular and irregular solutions of the free motion Schrödinger equation [8]

$$\begin{aligned} R_l(k, r) &\approx R_l^{\text{reg}}(k, r) - \tan \delta_l(k) R_l^{\text{irreg}}(k, r) \\ &= j_l(kr) - \tan \delta_l(k) n_l(kr) \\ &\sim \frac{1}{kr} \sin(kr - l\frac{\pi}{2} + \delta_l(k)), \end{aligned} \quad (30.1)$$

where the r.h.s. is valid when $r \rightarrow \infty$ and $\delta_l(k)$ is a phase shift in the l th partial wave induced by the potential $V(r)$. Our aim here is to calculate the phase shift in a framework of the harmonic oscillator representation. However before we do it, it is necessary to discuss how the phase shift can be introduced into the asymptotic expression ($n \gg 1$) of the wave function (30.1) taken in the harmonic oscillator representation, i.e., in correspondence with (28.4) and (28.6).

$$R_l(k, r) = \sum_n (-1)^n C_{nl}(k) R_{nl}(r), \quad (30.2a)$$

where

$$C_{nl}(k) = (-1)^n \int_0^\infty R_{nl}(r) R_l(k, r) r^2 dr, \quad (30.2b)$$

where in turn $C_{nl}(k)$ is a solution of Eq. (28.10).

It is clear that in the external region ($n \geq N$), where the contributions of the potential energy are negligible, this function also is a linear combination of the regular (29.6) and irregular (29.9) solutions of the equation (28.10c) so the relation between the coefficients is

$$C_{nl}(k) = C_{nl}^{\text{reg}}(k) - \tan \tilde{\delta}_l(k) C_{nl}^{\text{irreg}}(k). \quad (30.3)$$

Below we shall demonstrate that the factor $\tan \tilde{\delta}_l(k)$ of $C_{nl}^{\text{irreg}}(k)$ coincides with the corresponding factor $\tan \delta_l(k)$ in Eq. (30.1), i.e., $\tilde{\delta}_l(k) = \delta_l(k)$. For this aim, it is necessary to consider the behaviour of the integral (30.2b) at $n \gg 1$. It is more convenient to do it using the functions $R_l(k, r)$ and $R_{nl}(r)$ in the momentum representation

$$C_{nl}(k) = (-1)^n \int_0^\infty \tilde{R}_{nl}(q) \tilde{R}_l(k, q) q^2 dq, \quad (30.4)$$

where we use the tilde \sim to make clear the difference when dealing in ordinary or momentum space. It is useful to remember that wave functions $R_l(r)$ and $\tilde{R}_l(q)$ taken in the coordinate and momentum representations respectively, are connected with each other by the relations [11]

$$R_l(r) = \sqrt{\frac{2}{\pi}} \int_0^\infty \tilde{R}_l(q) j_l(qr) q^2 dq, \quad (30.5)$$

$$\tilde{R}_l(q) = \sqrt{\frac{2}{\pi}} \int_0^\infty R_l(r) j_l(qr) r^2 dr. \quad (30.6)$$

The spherical Bessel functions are normalized by the condition

$$\int_0^\infty j_l(qr) j_l(q'r) r^2 dr = \frac{\pi}{2q^2} \delta(q - q'), \quad (30.7a)$$

which follows from the plane wave normalization condition [10]

$$\begin{aligned} \langle \mathbf{q}' | \mathbf{q} \rangle &= \delta(\mathbf{q} - \mathbf{q}') = \frac{1}{q^2} \delta(q - q') \sum_{lm} Y_{lm}^*(\hat{\mathbf{q}}) Y_{lm}(\hat{\mathbf{q}}') \\ &= \frac{2}{\pi} \sum_{lm} \int_0^\infty j_l(q'r) j_l(qr) r^2 dr Y_{lm}^*(\hat{\mathbf{q}}) Y_{lm}(\hat{\mathbf{q}}'). \end{aligned} \quad (30.7b)$$

According to Eq. (29.5) the radial harmonic oscillator wave function $\tilde{R}_{nl}(k)$ in the momentum representation is equal to $(-1)^n R_{nl}(k)$. Using the asymptotic relation (29.7) we can rewrite the integral (30.4) in a form

$$\begin{aligned} C_{nl}(k) &\simeq \frac{2\sqrt{2}n^{1/4}}{\sqrt{\pi}} \int_0^\infty j_l(2\sqrt{n}q) \tilde{R}_l(k, q) q^2 dq \\ &= 2n^{1/4} R_l(k, 2\sqrt{n}), \quad n \gg 1. \end{aligned} \quad (30.8)$$

In the last line of this equation the formula (30.5) was used. We conclude that in the asymptotic region of $n \gg 1$ the scattering wave function $C_{nl}(k)$ in the harmonic oscillator representation is proportional to the corresponding coordinate wave function $R_l(k, r)$ with the argument r substituted by the value $2\sqrt{n}$. It should be noted that $2\sqrt{n}$ is the classical turning point in the three-dimensional harmonic oscillator potential for the energy $E_{nl} = 2n + l + \frac{3}{2} \approx 2n$. Equation (30.8) was established first by G.F. Filippov [2] using semiclassical arguments. We have used above the momentum representation (30.4) for $C_{nl}(k)$, which is convenient for the reason that the scattering wave function $\tilde{R}_l(k, q)$ for the particle with the momentum k , taken in a momentum representation, is concentrated in a narrow region of q close to $q = k$. Therefore it is always possible to substitute $\tilde{R}_{nl}(q)$ in (30.4) by its asymptotic form (29.7) in the interval of q , which is essential for the integration in (30.4), if the value of n is large.

Substituting the asymptotic expression (30.1) of $R_l(k, r)$ into the r.h.s. of Eq. (30.8) we obtain

$$C_{nl}(k) \approx 2n^{1/4} (j_l(2\sqrt{n}k) - \tan \delta_l(k) n_l(2\sqrt{n}k)). \quad (30.9)$$

The comparison of this result with Eq. (30.3) allows us to conclude that

$$\tilde{\delta}_l(k) = \delta_l(k). \quad (30.10)$$

Thus we obtain that the expression

$$C_{nl}(k) = C_{nl}^{\text{reg}}(k) - \tan \delta_l(k) C_{nl}^{\text{irreg}}(k) \quad (30.11)$$

is valid in the external region, i.e., at all $n \geq N + 1$ where Eq. (28.10c) is satisfied.

However, when $n = N + 1$ Eq. (28.10b) gives

$$\begin{aligned} &-T_{N+1N}^l C_{Nl}(k) + (T_{N+1N+1}^l - E) C_{N+1l}(k) \\ &- T_{N+1N+2}^l C_{N+2l}(k) = 0. \end{aligned} \quad (30.12)$$

It follows that the coefficient $C_{Nl}(k)$ has the same form (30.11),

$$C_{Nl}^{\text{ext}}(k) = C_{Nl}^{\text{reg}}(k) - \tan \delta_l(k) C_{Nl}^{\text{irreg}}(k), \quad (30.13)$$

as the expression (30.11) is valid for $C_{N+1l}(k)$ and $C_{N+2l}(k)$.

As the derivation was carried out coming from the external region $n > N$, we have put the symbol “ext” on the upper part of $C_{Nl}(k)$.

Alternative expression for the $C_{Nl}(k)$ coming from the inner part can be found using Eq. (28.10a).

Combining these two expressions,

$$C_{Nl}^{\text{ext}}(k) = C_{Nl}^{\text{inner}}(k), \quad (30.14)$$

we shall find the explicit formula for the calculation of the phase shift $\delta_l(k)$. Thus Eq. (30.14) plays the role of the fitting condition of the solutions of Eqs. (28.10) found in the internal and external regions.

Concerning Eq. (28.10a) it should be noted that they form a set of $N+1$ inhomogeneous linear equations of the form

$$\begin{aligned} \sum_{n=0}^N & \left((-1)^{n'-n} H_{n'n} - \delta_{n'n} E \right) C_{nl}(k) \\ & = \delta_{n'N} T_{NN+1}^l C_{N+1l}(k), \quad n' = 0, 1, \dots, N. \end{aligned} \quad (30.15)$$

In order to solve this set of equations it is reasonable to solve first the corresponding homogeneous set of equations omitting the term $T_{NN+1}^l C_{N+1l}(k)$ in r.h.s. of the last ($n' = N$) equation (30.15). The secular equation becomes

$$\det \left| (-1)^{n'-n} H_{n'n} - \delta_{n'n} E \right| = 0, \quad n', n = 0, 1, \dots, N, \quad (30.16)$$

giving the eigenvalues E_λ , $\lambda = 0, 1, 2, \dots, N$ and the corresponding orthonormal eigenvectors

$$\psi_\lambda = \sum_{n=0}^N \Gamma_{\lambda n} |nlm\rangle. \quad (30.17)$$

The coefficients $\Gamma_{\lambda n}$ form an unitary matrix Γ :

$$\sum_n \Gamma_{\lambda' n}^* \Gamma_{\lambda n} = \delta_{\lambda \lambda'}, \quad (30.18a)$$

$$\sum_\lambda \Gamma_{\lambda n'}^* \Gamma_{\lambda n} = \delta_{n'n}, \quad (30.18b)$$

and satisfy the equations

$$\sum_{n=0}^N \left((-1)^{n'-n} H_{n'n} - \delta_{n'n} E_\lambda \right) \Gamma_{\lambda n} = 0. \quad (30.18c)$$

Let us take Eq. (30.15) in a matrix form:

$$(\mathbf{H} - EI) \begin{pmatrix} C_{0l} \\ \vdots \\ \cdots \\ \cdots \\ C_{Nl} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \cdots \\ 0 \\ T_{NN+1}^l C_{N+1l} \end{pmatrix}, \quad (30.19)$$

where the matrix \mathbf{H} consists from the elements $(-1)^{n'-n} H_{n'n}$. Multiplying both sides of this equation by the matrix $\Gamma = |\Gamma_{\lambda n}|$ diagonalizing the $(N+1) \times (N+1)$ truncated Hamiltonian matrix \mathbf{H} ,

$$\Gamma \mathbf{H} \Gamma^\dagger = \begin{pmatrix} E_0 & 0 & \dots & 0 \\ 0 & E_1 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & E_N \end{pmatrix}, \quad (30.20)$$

we obtain

$$(E_\lambda - E) \sum_{n=0}^N \Gamma_{\lambda n} C_{nl}(k) = T_{NN+1}^l \Gamma_{\lambda N} C_{N+1l}(k), \quad \lambda = 0, 1, \dots, N, \quad (30.21a)$$

or

$$\sum_{n=0}^N \Gamma_{\lambda n} C_{nl}(k) = \frac{T_{NN+1}^l \Gamma_{\lambda N}}{E_\lambda - E} C_{N+1l}(k). \quad (30.21b)$$

The multiplication of both sides of this equation by $\Gamma_{\lambda n'}^*$ and summation on λ gives the result

$$C_{n'l}(k) = \sum_\lambda \frac{\Gamma_{\lambda n'}^* \Gamma_{\lambda N}}{E_\lambda - E} T_{NN+1}^l C_{N+1l}(k) \quad (30.22)$$

if the property (30.18b) is taken into account.

This relation gives an expression for arbitrary “internal” coefficients $C_{nl}(k)$ ($n \leq N$) in terms of the “external” coefficient $C_{N+1l}(k)$:

$$C_{nl}(k) = \varrho_{nN+1} C_{N+1l}(k), \quad (30.23)$$

where

$$\varrho_{nN+1} = T_{NN+1}^l \sum_\lambda \frac{\Gamma_{\lambda n}^* \Gamma_{\lambda N}}{E_\lambda - E}. \quad (30.24)$$

In the particular case of $n = N$ we have

$$C_{Nl}^{\text{inner}}(k) = \varphi_{NN+1} C_{N+1l}(k). \quad (30.25)$$

If we substitute the expressions (30.13), (30.25) and (30.11) into the "fitting condition" (30.14) we find

$$C_{Nl}^{\text{reg}}(k) - \tan \delta_l(k) C_{Nl}^{\text{irreg}}(k) = \varphi_{NN+1} \left(C_{N+1l}^{\text{reg}}(k) - \tan \delta_l(k) C_{N+1l}^{\text{irreg}}(k) \right).$$

Thus,

$$\tan \delta_l(k) = \frac{C_{Nl}^{\text{reg}}(k) - \varphi_{NN+1} C_{N+1l}^{\text{reg}}(k)}{C_{Nl}^{\text{irreg}}(k) - \varphi_{NN+1} C_{N+1l}^{\text{irreg}}(k)}, \quad (30.26)$$

where

$$\varphi_{NN+1} = \sum_{\lambda} T_{NN+1}^l \frac{|\Gamma_{\lambda N}|^2}{E_{\lambda} - E}. \quad (30.27)$$

Because $C_{nl}^{\text{reg}}(k)$ and $C_{nl}^{\text{irreg}}(k)$ are known for all values of n , it is clear that the formulae (30.26) and (30.27) allow to find the approximate values of phase shifts $\delta_l^N(k)$ at an arbitrary energy $E = k^2/2$ by diagonalizing a (large) matrix only once. (Here we add an upper N to indicate the number of quanta when the potential was cut). The improvement of the results can be reached by increasing the size of the truncated Hamiltonian matrix H . The calculations should be stopped when approximate phase shifts $\delta_l^N(k)$ and $\delta_l^{N+1}(k)$ will coincide within the necessary precision in the energy region under consideration.

In agreement with the Ritz variational principle the negative eigenvalues $E_{\lambda} < 0$ of the truncated Hamiltonian matrix H may be treated as approximate values of the energies of discrete levels in the potential studied. Also in this case the accuracy of the approximation is improved by increasing the size of the matrix H . The question arises: What is the sense of the positive eigenvalues of the truncated matrix H and of the corresponding wave functions? The question is answered as follows: In the limit $E \rightarrow E_{\lambda}$ the expression (30.26) takes the form

$$\tan \delta_l(E_{\lambda}) = \frac{C_{N+1l}^{\text{reg}}(E_{\lambda})}{C_{N+1l}^{\text{irreg}}(E_{\lambda})}. \quad (30.28)$$

Comparing this result with the formula (30.11) we get the coefficient

$$C_{N+1l}(k) = 0 \quad (30.29)$$

at $E = E_{\lambda}$. Thus, by diagonalizing the Hamiltonian matrix H we find the solutions of Eqs. (28.10) at such discrete energies E_{λ} which correspond to

31. EXACTLY SOLUBLE EXAMPLE

the vanishing of $C_{nl}(E_{\lambda})$ at the point $n = N + 1$. If $E_{\lambda} > 0$ the scattering phase shifts are calculated at such energies using the simple formula (30.28).

31 Exactly Soluble Example

As an illustration of the approach to the calculation of the phase shift, described above, let us consider the s -wave scattering problem for smooth central potential $V(r)$, taken in a lowest approximation ($N = 0$). It means that the Hamiltonian $H = T + V$ is approximated by the matrix with elements

$$H_{nn'} = T_{nn'}^0, \quad (31.1)$$

except for

$$H_{00} = T_{00}^0 + V_0, \quad (31.2a)$$

where

$$V_0 = \langle 000 | V(r) | 000 \rangle. \quad (31.2b)$$

The first step to the calculation of the phase shift is a diagonalization of the truncated Hamiltonian matrix H^N . In our case of $N = 0$ it is superfluous because we have a matrix of a size 1×1 . Its single eigenvalue in our units $\hbar = m = \omega = 1$ is equal to

$$E_0 = \langle 000 | H | 000 \rangle = T_{00}^0 + V_0; \quad T_{00}^0 = \frac{3}{4}, \quad (31.3)$$

and the corresponding eigenfunction coincides with $|000\rangle$, i.e., $\Gamma_{00} = 1$ in the formulae (30.21), (30.22) and (30.27). Thus,

$$\varphi_{01} = T_{01}^0 \frac{\Gamma_{00}^2}{E_0 - E} = \frac{\sqrt{3}}{2\sqrt{2}} \frac{1}{\frac{3}{4} + V_0 - E}. \quad (31.4)$$

Now, using the formula (30.26) we obtain

$$\tan \delta_0(k) = \frac{C_{00}^{\text{reg}}(k) - \varphi_{01} C_{10}^{\text{reg}}(k)}{C_{00}^{\text{irreg}}(k) - \varphi_{01} C_{10}^{\text{irreg}}(k)}. \quad (31.5)$$

In order to find the phase shift in an analytical form the explicit expressions of the coefficients C_{00}^{reg} , C_{10}^{reg} , C_{00}^{irreg} and C_{10}^{irreg} should be substituted to Eq. (31.5).

At first we consider the numerator of this equation. Using Eq. (28.10c) which takes the form

$$(T_{00}^0 - E) C_{00}^{\text{reg}}(k) - T_{01}^0 C_{10}^{\text{reg}}(k) = 0; \quad (31.6)$$

in our case, using (29.6), we can write

$$\begin{aligned} & C_{00}^{\text{reg}}(k) + \frac{T_{01}^0}{E-E_0} C_{10}^{\text{reg}}(k) \\ &= \frac{C_{00}^{\text{reg}}(k)(E-T_{00}^0-V_0)+T_{01}^0 C_{10}^{\text{reg}}(k)}{(E-E_0)} \\ &= -\frac{V_0}{E-E_0} C_{00}^{\text{reg}}(k) = \left(\frac{2V_0}{\pi^{1/4}} e^{-k^2/2} \right) / \left(\frac{3}{4} - \frac{k^2}{2} + V_0 \right). \end{aligned} \quad (31.7)$$

As for the denominator of Eq. (31.5), the coefficient

$$C_{10}^{\text{irreg}}(k) = -\frac{2\sqrt{2}}{\sqrt{3}\pi^{3/4}k} e^{-k^2/2} M\left(-\frac{3}{2}, \frac{1}{2}; k^2\right) \quad (31.8a)$$

can be expressed in terms of the coefficient

$$C_{00}^{\text{irreg}}(k) = -\frac{2}{k\pi^{3/4}} e^{-k^2/2} M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right) \quad (31.8b)$$

using the properties of confluent hypergeometric functions. Let us recall at first the explicit expressions for some particular cases of the confluent hypergeometric function taken from reference [7]:

$$M\left(\frac{1}{2}, \frac{1}{2}; k^2\right) = e^{k^2}, \quad (31.9)$$

$$M\left(\frac{1}{2}, \frac{3}{2}; k^2\right) = i\frac{\sqrt{\pi}}{2k} \operatorname{erf}(-ik). \quad (31.10)$$

These results allow to find $M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right)$ using the recurrent relation [7]

$$bM(a, b, z) - bM(a-1, b, z) - zM(a, b+1, z) = 0, \quad (31.11)$$

which gives (at $a = b = 1/2$, $z = k^2$) an expression of $C_{00}^{\text{irreg}}(k)$ in terms of error function

$$M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right) = e^{k^2} - i\sqrt{\pi}k \operatorname{erf}(-ik). \quad (31.12)$$

The recurrence relation [7]

$$(b-a)M(a-1, b, z) + (2a-b+z)M(a, b, z) - aM(a+1, b, z) = 0 \quad (31.13)$$

gives us the possibility to express $M\left(-\frac{3}{2}, \frac{1}{2}; k^2\right)$ in terms of $M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right)$, i.e,

$$-M\left(-\frac{3}{2}, \frac{1}{2}; k^2\right) = \frac{1}{2}e^{k^2} - \left(\frac{3}{2} - k^2\right)M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right). \quad (31.14)$$

Because of this property we have

$$\begin{aligned} & C_{10}^{\text{irreg}}(k) \\ &= \frac{2\sqrt{2}}{\sqrt{3}\pi^{3/4}k} \left\{ \frac{1}{2}e^{k^2/2} - \left(\frac{3}{2} - k^2\right) e^{-k^2/2} M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right) \right\} \\ &= \sqrt{\frac{2}{3}} \frac{1}{\pi^{3/4}k} e^{k^2/2} + \sqrt{\frac{2}{3}} \left(\frac{3}{2} - k^2\right) C_{00}^{\text{irreg}}(k). \end{aligned} \quad (31.15)$$

The substitution of this expression into the denominator of Eq. (31.5) gives ($E = k^2/2$)

$$\begin{aligned} & C_{00}^{\text{irreg}}(k) - \rho_{01} C_{10}^{\text{irreg}}(k) \\ &= \left[\left(\frac{3}{4} - \frac{k^2}{2} + V_0 \right) C_{00}^{\text{irreg}}(k) - \frac{\sqrt{3}}{2\sqrt{2}} \cdot \sqrt{\frac{2}{3}} \frac{1}{\pi^{3/4}k} e^{k^2/2} \right. \\ &\quad \left. - \frac{\sqrt{3}}{2\sqrt{2}} \cdot \sqrt{\frac{2}{3}} \left(\frac{3}{2} - k^2\right) C_{00}^{\text{irreg}}(k) \right] / \left[\frac{3}{4} - \frac{k^2}{2} + V_0 \right] \\ &= - \left[\frac{1}{2\pi^{3/4}k} e^{k^2/2} - V_0 C_{00}^{\text{irreg}}(k) \right] / \left[\frac{3}{4} - \frac{k^2}{2} + V_0 \right] \\ &= - \left[\frac{1}{2\pi^{3/4}k} e^{k^2/2} + V_0 \frac{2}{\pi^{3/4}k} e^{-k^2/2} M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right) \right] \\ &\quad \times \left[\frac{3}{4} - \frac{k^2}{2} + V_0 \right]^{-1} \\ &= -\frac{1}{2\pi^{3/4}k} e^{k^2/2} \left(1 + 4V_0 e^{-k^2} M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right) \right) \\ &\quad \times \left[\frac{3}{4} - \frac{k^2}{2} + V_0 \right]^{-1}. \end{aligned} \quad (31.16)$$

Combining this formula with Eq. (31.7) we obtain the final result

$$\tan \delta_0(k) = -\frac{4\sqrt{\pi}kV_0 e^{-k^2}}{1 + 4V_0 e^{-k^2} M\left(-\frac{1}{2}, \frac{1}{2}; k^2\right)}. \quad (31.17)$$

Thus we have all necessary and sufficient information in order to calculate the phase shift for our simple problem and to discuss its peculiarities.

We begin with a discussion of bound state in the potential represented by the matrix (31.2).

It is well known that the bound states correspond to the poles of S -matrix on the positive imaginary axis in the complex k plane. Each such pole $k = i\alpha$ generates a bound state with a binding energy $E_B = \alpha^2/2$.

As for the S -matrix, it can be expressed in terms of $\tan \delta$ as follows:

$$S(k) = e^{2i\delta(k)} = \frac{1 + i \tan \delta(k)}{1 - i \tan \delta(k)}. \quad (31.18)$$

The substitution of the result (31.17) into this formula gives

$$S = \frac{1 + 4V_0 \left(1 - i\sqrt{\pi}ke^{-k^2} \operatorname{erfc}(ik) \right)}{1 + 4V_0 \left(1 + i\sqrt{\pi}ke^{-k^2} \operatorname{erfc}(-ik) \right)}. \quad (31.19)$$

Thus the equation, determining the S -matrix pole(s), corresponding to the bound state(s), is of the form

$$1 + 4V_0 \left(1 - \alpha\sqrt{\pi}e^{\alpha^2} \operatorname{erfc} \alpha \right) = 0. \quad (31.20)$$

The expression in brackets is positive. Therefore the Hamiltonian (31.1) possesses a bound state only at negative amplitude

$$V_0 \leq -\frac{1}{4}. \quad (31.21)$$

Since the function $\alpha e^{\alpha^2} \operatorname{erfc} \alpha$ increases monotonically [7] from 0 to $1/\sqrt{\pi}$ with the growth of α only one bound state exists in a system with the Hamiltonian (31.1) if the condition (31.21) is satisfied. The dependence of the phase shift (31.8) on the momentum k is given at Fig. VI.1 for positive (curve 1) and negative (curves 2 and 3) amplitudes V_0 . In correspondence with the Levinson theorem [12] the phase shift $\delta_0(k)$ falls down from π to 0 when the condition (31.21) of the existence of the bound state is satisfied (curve 3). It is interesting that at positive amplitude V_0 the phase shift $\delta_0(k)$ falls down linearly:

$$\tan \delta_0(k) \simeq -ka, \quad k \sim 0, \quad (31.22)$$

similarly to the phase shift for the scattering on the repulsive core potential with a radius $a = 4\sqrt{\pi}V_0/(1 + 4V_0)$.

32 Phase Shift and Resonances in the Harmonic Oscillator Representation

a) s -scattering on the Gaussian potential

As an example of the phase shift calculations in the harmonic oscillator representation we consider the s -scattering on the Gaussian potential $V(r) =$

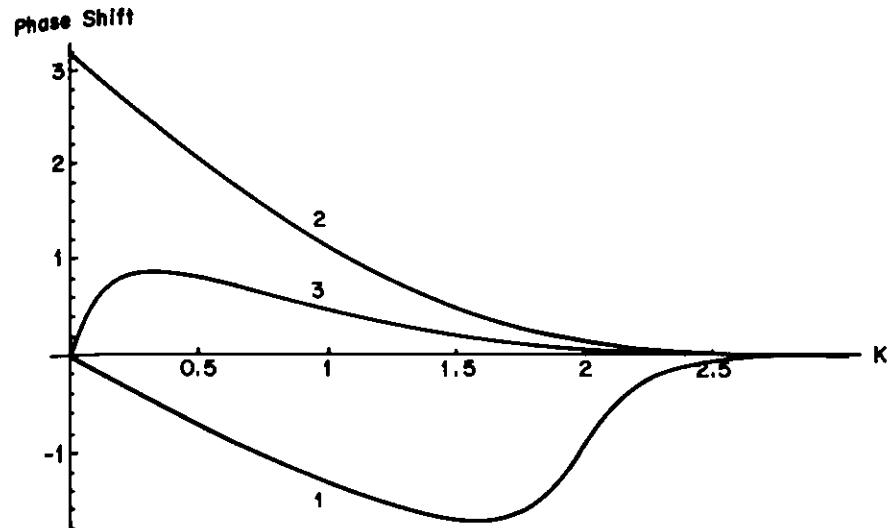


Figure VI.1. The phase shift $\delta_0(k)$ for the Hamiltonian (31.2). The curves 1,2 and 3 correspond to the values $V_0 = 1.0, -1.0$ and -0.2 respectively.

$V_0 \exp(-\gamma r^2)$ with parameters $V_0 = -4.2$, $\gamma = 0.22$ that are typical for nuclear systems if we use units in which $\hbar = m = \omega = 1$ while $\hbar\omega \approx 16$ MeV and m is the nucleon mass. The matrix elements of the Gauss potential can be calculated by the procedure described in the Section 2. The approximate calculation of the phase shift is made using the formula (30.26) at $N=3,5$ and 9. The exact values of the phase shift $\delta_0(k)$ are found numerically by the phase function method [13]. The results of the s -wave phase shift calculations are presented at Fig. VI.2. It is clear from this picture that the choice of the truncation boundary $N \simeq 10$ gives stable results for the phase shift $\delta_0(k)$ at energies $E \leq 5$ (it corresponds about 70 MeV for the nucleon scattering on light nuclei). This example shows that the convergence of our approach in practical calculations is rather good.

b) s -scattering on the δ -shell potential

As a second example we consider the s -scattering on the δ -shell potential [6,14,15]:

$$V(r') = b\delta(r' - a). \quad (32.1)$$

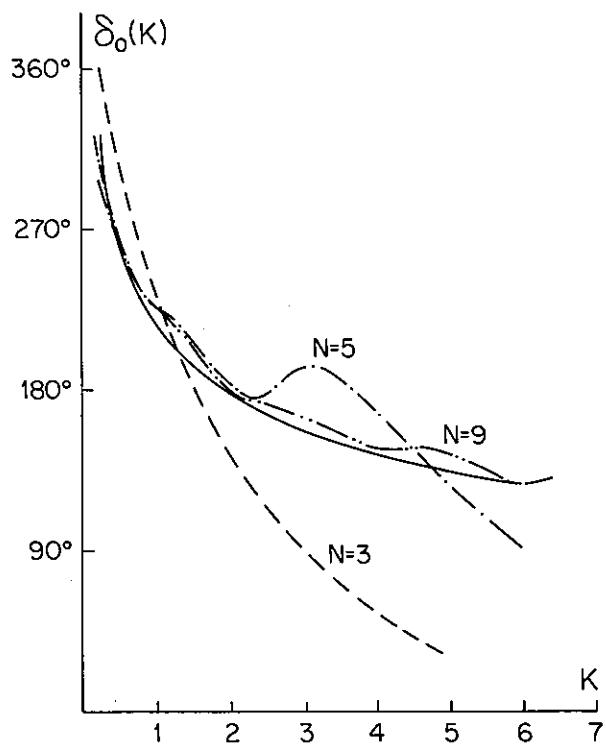


Figure VI.2. The phase shift $\delta_0^N(\kappa)$ for the Gaussian potential ($V_0 = -4.2$, $\gamma = 0.22$) calculated in the harmonic oscillator representation at various values of N . The solid curve presents the results of exact numerical calculations.

The Schrödinger equation for this potential in normal unit, and using the notation (3.1), becomes

$$\left(\frac{p'^2}{2m} + b\delta(r' - a) \right) \Psi(r') = E\Psi(r'), \quad (32.2)$$

and it can be solved analytically. It allows us to do a more detailed analysis of the convergence of the approach described at the Section 30. If we restrict ourselves by the s -scattering and introduce a new function $\chi(r') = r'\Psi(r')$ the last one satisfies the equation

$$-\frac{d^2\chi}{dr'^2} + g\delta(r' - a)\chi = k^2\chi, \quad (32.3a)$$

where

$$g = \frac{2mb}{\hbar^2} \text{ and } E = \frac{\hbar^2 k^2}{2m}. \quad (32.3b)$$

Equation (32.3a) is solved with the boundary condition $\chi(0) = 0$. In the inner region the solution is of the form

$$\chi_{\text{int}}(r') = \sin kr', \quad 0 \leq r' \leq a. \quad (32.4)$$

In the external region we have

$$\chi_{\text{ext}}(r') = B \sin(kr' + \delta), \quad r' \geq a. \quad (32.5)$$

The coefficient B and the phase shift $\delta(k)$ can be found by fitting of the inner and external parts of the wave function and their derivatives in the barrier point $r' = a$. The continuity condition of the wave function

$$\chi_{\text{int}}(a) = \chi_{\text{ext}}(a)$$

gives the relation

$$\sin ka = B \sin(ka + \delta). \quad (32.6)$$

The condition for the derivatives can be found as follows. Let us integrate both sides of Eq. (32.3a) on r' at the interval $(a - \Delta, a + \Delta)$, obtaining

$$-\left. \frac{d\chi}{dr'} \right|_{a+\Delta} + \left. \frac{d\chi}{dr'} \right|_{a-\Delta} + g\chi(a) = k^2 \int_{a-\Delta}^{a+\Delta} \chi(r') dr'. \quad (32.7)$$

In the limit $\Delta \rightarrow 0$ it gives

$$\left(\frac{d\chi_{\text{ext}}}{dr'} \right)_{r'=a} - \left(\frac{d\chi_{\text{int}}}{dr'} \right)_{r'=a} = g\chi(a), \quad (32.8)$$

i.e., the logarithmic derivative of the wave function $\chi(r')$ has a positive jump g at the barrier. It means that

$$\cot(ka + \delta) = \cot ka + \frac{g}{k}. \quad (32.9)$$

The phase shift can be found from this relation as

$$\delta(ka) = -ka + \arctan \left(\frac{ka \tan ka}{ka + ga \tan ka} \right). \quad (32.10)$$

As for the coefficient B it is equal to

$$B = \frac{\sin(ka + \delta)}{\sin ka}. \quad (32.11)$$

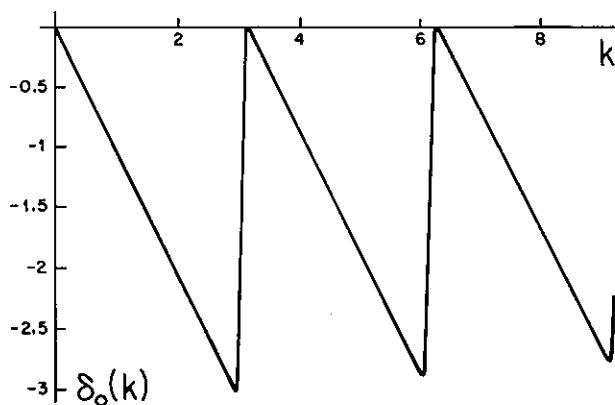


Figure VI.3. The phase shift $\delta_0(k)$ for the δ -shell potential (32.1) at $g = 100$.

The dependence of the phase shift on the wave vector (momentum) k is shown at Fig. VI.3 ($g = 100$).

It should be noted that δ vanishes at $k = \nu\pi$ ($\nu = 0, 1, 2, \dots$). Therefore at corresponding energies the scattering (of the s -wave) is *absent*.

Now, after the main characteristics of the s -scattering on the potential (32.1) are found analytically let us consider what results for the phase shift $\delta(k)$ can be obtained using the formula (30.26).

The matrix elements of the Hamiltonian

$$H' = \frac{p'^2}{2m} + b\delta(x' - a) \quad (32.12)$$

in the harmonic oscillator basis can be found using the procedure described in the Section 3.

Make the change of variables

$$x_i = \sqrt{\left(\frac{m\omega}{\hbar}\right)} x'_i, \quad (32.13)$$

$$p_i = \frac{1}{\sqrt{m\omega\hbar}} p'_i, \quad (32.14)$$

$$H = \frac{H'}{E_0}, \quad (32.15)$$

where the value $E_0 = \hbar^2/2ma^2$ is connected with the energy E_1 of the lowest level in an infinite square well of the radius a by the relation

$$E_1 = \pi^2 E_0. \quad (32.16)$$

Define the dimensionless parameter

$$\varepsilon = \sqrt{\frac{\hbar\omega}{2E_0}} = a\sqrt{\frac{m\omega}{\hbar}}. \quad (32.17)$$

Then,

$$H = \varepsilon^2 p^2 + \beta\varepsilon\delta(r - \varepsilon), \quad (32.18)$$

where $\beta = 2mab/\hbar^2$.

The matrix elements of this Hamiltonian in the harmonic oscillator basis with a unit frequency are

$$\langle n'00 | H | n00 \rangle = \varepsilon^2 \langle n'00 | p^2 | n00 \rangle + \beta\varepsilon R_{n'0}(\varepsilon)R_{n0}(\varepsilon), \quad (32.19)$$

with

$$\begin{aligned} \langle n'00 | p^2 | n00 \rangle = \\ \sqrt{(n+1)(n+\frac{3}{2})} \delta_{n'n+1} + (2n+1) \delta_{n'n} + \sqrt{n(n+\frac{1}{2})} \delta_{n'n-1}. \end{aligned} \quad (32.20)$$

For the calculation of the phase shift δ it is necessary to find the eigenvalues $E_\lambda^{(N)}(\varepsilon)$ of the finite matrix H^N with matrix elements (32.19) ($n, n' \leq N$) by the diagonalization of this matrix and to obtain also the corresponding eigenvectors with components $C_{n\lambda}(\varepsilon)$ ($n = 0, 1, \dots, N$). Then the formula (30.26) should be used.

The numerical calculations of the phase shift $\delta(k)$ for the δ -shell potential by this method were done in ref. [6] at values of $N = 30$ and 80 and $\beta = 8$. A number of values of the parameter ε was used. The optimal convergence of the calculations was observed at $\varepsilon \approx 10$. The results of these calculations are presented at Fig. VI.4. Also the curve, corresponding to the exact values $\delta(k)$, is given. The comparison of the approximate phase shift $\delta^{(N)}(k)$ with the exact values $\delta(k)$ shows that a very good description of the exact phase shift can be obtained in the frame of the harmonic oscillator representation at rather modest value of $N \sim 75$.

c) Evidence of resonances in the variational calculations on the harmonic oscillator basis.

It is well known [6,14,15] that there are no bound states in the potential (32.1). However there is a number of sharp resonances if the amplitude b of the barrier is rather large. These resonances correspond to the S -matrix

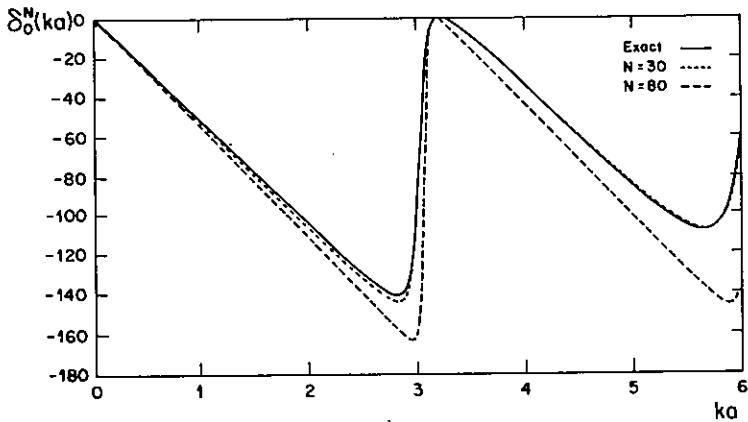


Figure VI.4. The convergence of the phase shift $\delta_0^N(\kappa)$ for the δ -shell potential ($g = 8$, $N = 30$ and 80). The solid curve shows the exact result. (It is taken from F. Arickx *et al.* in reference [6]).

poles. The number of these poles is infinite, but only the lowest poles close to the real energy axis generate noticeable maxima in the elastic scattering cross section $\sigma_{el} = (4\pi/k^2) \sin^2 \delta$. The advantage of the potential (32.1) is that the S -matrix poles can be found semi-analytically. Besides, as it was shown in the previous subsection, the calculation of the approximate values of the phase shift include the diagonalization of the Hamiltonian matrix H^N on the harmonic oscillator basis as an intermediate step. It allows us to analyze the connection between the eigenvalues $E_\lambda^{(N)}(\varepsilon)$, found in the variational calculations, and the characteristics of resonances (the poles of S -matrix) inherent to the scattering problem under consideration. In this connection we discuss below the correlation between the behaviour of the roots $E_\lambda^{(N)}(\varepsilon)$ of the secular equation for the potential (32.1) as a function of ε and the positions of resonances. As in the previous subsection we give at first the exact results for the resonance characteristics, then numerical calculations of $E_\lambda^{(N)}(\varepsilon)$ at rather large $N=24$ are described. As a conclusion the interrelation between $E_\lambda^{(N)}(\varepsilon)$ and resonance energies E_ν is discussed. The important feature is established in this analysis that the positive roots $E_\lambda^{(N)}(\varepsilon) > 0$ of the secular equation are monotonically increasing with a growth of ε in contradiction to the negative roots which, as it was demonstrated in Sections 3,4, have a minima as a function of ε . Although these conclusions are obtained for a particular type of the potential they are valid in a general case too.

32. PHASE SHIFT AND RESONANCES

It is well known [12] that the resonances in the elastic scattering are connected with poles of S -matrix

$$S = e^{2i\delta} \quad (32.21)$$

in a plane of complex momentum k . The relation (32.10) gives the following expression for the S -matrix:

$$S = e^{-2i(ka)} \frac{(ka \cot ka + ga) + ika}{(ka \cot ka + ga) - ika}. \quad (32.22)$$

The S -matrix poles are determined by the equation

$$\cot ka = -\frac{g}{k} + i,$$

or

$$\tan ka = \frac{k}{-g + ik}. \quad (32.23)$$

We are interested in the case of very narrow resonances arising at the condition

$$g \gg \frac{\pi\nu}{a}. \quad (32.24)$$

It follows from Eq. (32.23) that in this case the poles of the S -matrix appear near the points $\pi\nu/a$, *i.e.*,

$$k_\nu a = \pi\nu + \xi, \quad (32.25)$$

where $|\xi| \ll 1$. Conserving lowest terms in both sides of (32.23) we obtain [15]

$$\tan \xi \simeq \xi = -\frac{\pi\nu}{ga} - i \left(\frac{\pi\nu}{ga} \right)^2, \quad (32.26)$$

i.e.,

$$k_\nu a = \pi\nu \left(1 - \frac{1}{ga} \right) - i \left(\frac{\pi\nu}{ga} \right)^2 \simeq \pi\nu - i\gamma^2, \quad (32.27a)$$

$$\gamma^2 = \frac{\pi^2 \nu^2}{g^2 a^2}. \quad (32.27b)$$

For the resonance energy we have [15]

$$E = E_\nu - i\Gamma_\nu/2, \quad (32.28a)$$

$$E_\nu \simeq \frac{\pi^2 \nu^2 \hbar^2}{2ma^2}, \quad \Gamma_\nu = 2\pi\nu \frac{\hbar^2 \gamma^2}{ma^2} = \frac{(\pi\nu)^3}{g^2 a^2} \frac{\hbar^2}{ma^2}. \quad (32.28b)$$

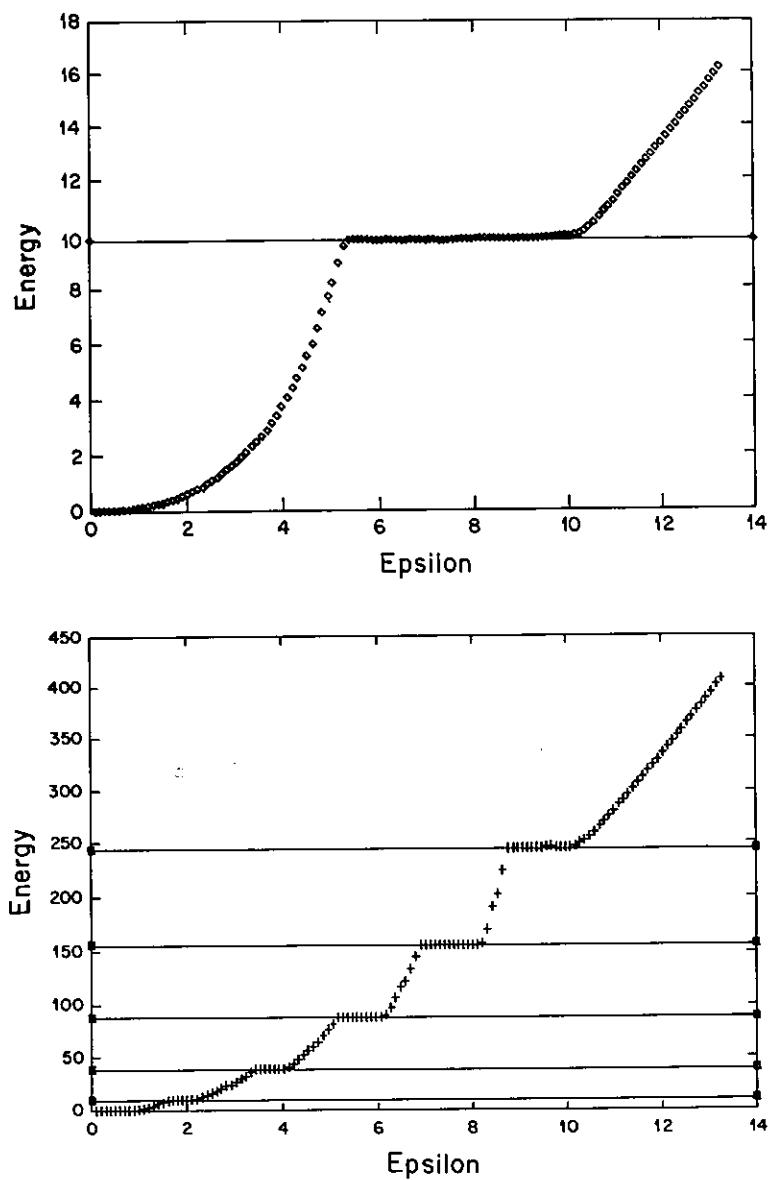


Figure VI.5 (top). The ϵ -dependence of the lowest eigenvalue $E_1^{(N)}$ of the secular equation (32.32) ($N = 24$).

Figure VI.6 (bottom). The ϵ -dependence of the fifth eigenvalue $E_5^{(N)}$ of the secular equation (32.32) ($N = 24$).

At $ga \gg \pi\nu$ the width Γ_ν of the resonance can be very small.

Now, when the characteristics of resonances in the s -wave scattering on the δ -shell potential are found, let us consider how these resonances can be visualized in the variational calculations on the harmonic oscillator basis.

The results of the diagonalization of the matrix H^N are presented in Figs. VI.5 and VI.6. In all cases the harmonic oscillator basis $|n00\rangle$ was used with $n = 0, 1, \dots, 24$. The harmonic oscillator frequency ω was applied as a nonlinear variational parameter (more correctly the abscissa axis corresponds to the parameter $\epsilon \sim \omega^{1/2}$ changing between 0 and 15). The amplitude of the δ -shell potential was taken rather high ($\beta = 100$) in order to have narrow resonances at small values of $\nu = 1, 2, \dots$

What features of these pictures should be remarked? At Fig. VI.5 the ω -dependence of the lowest (first) root $E_1^{(N)}$ of the secular equation is presented. It is seen that this root increases rapidly with a growth of ϵ (or ω) from zero at $\omega = 0$ up to the value $E_1 \sim 5 \hbar^2/ma^2$ at $\epsilon \approx 5$. Then the function $E_1^{(N)}(\epsilon)$ has a *plateau* between $\epsilon \approx 5$ and $\epsilon \approx 10$. The position of this plateau corresponds to the energy of the *first resonance* $E_1 \approx \pi^2 E_0$. At $\epsilon \approx 10$ the further (parabolic) increasing of $E_1^{(N)}(\epsilon)$ is observed when ϵ rises.

At Fig. VI.6 similar results for the fifth root $E_5^{(N)}(\epsilon)$ of the secular equation are presented. The general trend in its behaviour is the monotonic growth when ϵ increases. However in this case there are five plateaux. The first plateau is close to the energy of the first resonance $E_1 \approx \pi^2 E_0$, the second plateau is posed near the energy of the second resonance $E_2 \sim 4\pi^2 E_0$ etc. The last plateau position corresponds to the energy of the fifth resonance $E_5 \approx 25\pi^2 E_0$. In general the curve $E_\lambda^{(N)}(\epsilon)$ ($\lambda \leq N$) contains λ plateaux corresponding to the resonances E_s ($s = 1, 2, \dots, \lambda$). The questions arise: what is a reason of the appearance of such plateaux and why their positions are correlated with the resonance energies? The answers to these questions can be found in the following way. As it was mentioned at the end of the Section 30, the diagonalization of the H^N is equivalent to the solution of the equations (28.10) at the boundary condition

$$C_{N+1}(k) = 0. \quad (32.29)$$

In accordance with (30.8), the coefficients $C_n(k)$ at $n \gg 1$ are proportional to the configuration space wave function $R(k, r')$, with r' substituted by $2\sqrt{n}a/\epsilon$:

$$C_n(k) \approx \chi \left(2\sqrt{n} \frac{a}{\epsilon} \right). \quad (32.30)$$

In correspondence with the expressions (32.4) and (32.5) it means that

$$C_n(k) \sim \sin\left(\frac{2ka\sqrt{n}}{\varepsilon}\right), \quad \frac{2\sqrt{n}}{\varepsilon} < 1, \quad (32.31a)$$

$$C_n(k) \sim \sin\left(\frac{2ka\sqrt{n}}{\varepsilon} + \delta(k)\right), \quad \frac{2\sqrt{n}}{\varepsilon} > 1. \quad (32.31b)$$

Equation (32.31a) takes place only for the δ -shell potential while the second relation (32.31b) is valid for the arbitrary short-range potential of radius a .

Thus the behaviour of the roots $E_\lambda^{(N)}(\varepsilon)$ of the secular equation

$$\det |H^N - E| = 0 \quad (32.32)$$

as a function of ε can be understood if we find the solutions k_ν of Eq. (32.29):

$$\sin\left(\frac{2ka\sqrt{N}}{\varepsilon}\right) = 0, \quad \varepsilon \geq 2\sqrt{N}, \quad (32.33a)$$

$$\sin\left(\frac{2ka\sqrt{N}}{\varepsilon} + \delta(k)\right) = 0, \quad \varepsilon \leq 2\sqrt{N}, \quad (32.33b)$$

because the phase shift $\delta(k)$ for the δ -shell potential was studied in the previous subsection.

The solution of Eq. (32.33a) is equal to

$$k_\nu = \frac{\pi\nu\varepsilon}{2a\sqrt{N}}, \quad (32.34)$$

i.e., the momentum k_ν rises linearly with ε with increasing of $\varepsilon > 2\sqrt{N}$. The corresponding eigenvalue $E_\lambda^{(N)}(\varepsilon) = \hbar^2 k_\nu^2 / 2m$ increases parabolically with a growth of $\varepsilon > 2\sqrt{N}$. It is clear that ν coincides with the order number of the root $E_\lambda^{(N)}(\varepsilon)$ in the region $\varepsilon > 2\sqrt{N}$. If $\varepsilon < 2\sqrt{N}$ the equation (32.33b) gives

$$\frac{2ka\sqrt{N}}{\varepsilon} + \delta(k) = \pi\nu, \quad \nu = 1, 2, \dots \quad (32.35)$$

The last transcendent equation can be solved by graphic method as it is shown in Fig. VI.7. In this picture the zig-zag line, consisting of the sections OA, AB, BC, CD, ..., represents (schematically) the $\delta(ka)$ of Eq. (32.10) and thus (32.35) can be written as

$$\pi\nu - \frac{ka}{\alpha} = \delta(ka), \quad (32.36)$$

with $\alpha = \varepsilon/2\sqrt{N}$.

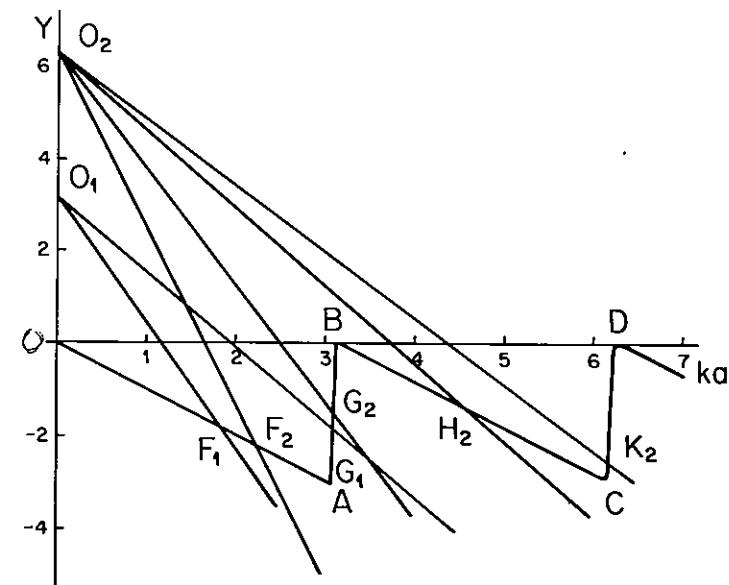


Figure VI.7. The graphic solution of the transcendental Eq. (32.35).

The straight lines of the type $O_1F_1, O_1G_1, O_2F_2, O_2G_2, O_2H_2, O_2K_2, \dots$, correspond to the l.h.s.

$$y(ka) = \pi\nu - \frac{ka}{\alpha} \quad (32.37)$$

of Eq. (32.36). (In Fig. VI.7 only straight lines with $\nu = 1$ and 2 are given.) The slopes of these lines are regulated by the parameter α (or ε)

The angle between such a line and the ordinate axis changes from 0 up to $\frac{\pi}{4}$ when α runs between 0 and 1. (It should be noted that similarly to (32.31b), (32.36) is valid when $0 < \varepsilon < 2\sqrt{N}$ or $0 \leq \alpha \leq 1$.)

The abscissas of crossing points (of the type $F_1, G_1, F_2, G_2, H_2, K_2, \dots$) of the straight lines (32.37) with the zig-zag line, approximating the function $\delta(ka)$, give the solutions $k_\nu a(\alpha)$ (or $k_\nu(\varepsilon)$) of Eq. (32.36).

Let us consider, for example, the ε -dependence of the lowest solution $k_1(\varepsilon)$ (i.e., $\nu = 1$) of Eq. (32.35). It is clear from Fig. VI.7 that the straight line $y = \pi - \frac{ka}{\alpha}$ crosses the piece OA of the zig-zag line, in which

$$\delta(ka) \simeq -ka \quad (32.38)$$

at the value which we denote as

$$k_1 a = \frac{\pi\alpha}{(1-\alpha)}. \quad (32.39)$$

When the crossing point F_1 coincides with the end A of the first zig-zag line section OA the value of parameter α is equal to $\frac{1}{2}$. Thus the ε dependence of the lowest solution of Eq. (32.35) is described by the hyperbola

$$k_1(\varepsilon) = \frac{\pi\varepsilon}{a(2\sqrt{N} - \varepsilon)} = \frac{\pi}{a} \left(-1 + \frac{2\sqrt{N}}{2\sqrt{N} - \varepsilon} \right) \quad (32.40)$$

at the interval $0 < \varepsilon < \sqrt{N}$ ($0 < \alpha < \frac{1}{2}$). When the parameter α runs between $\frac{1}{2}$ and 1 ($\sqrt{N} < \varepsilon < 2\sqrt{N}$) the crossing point G_1 of the line (32.37) and the second piece AB of the broken line has a constant abscissa $x_1 \simeq \pi$. It means that the lowest solution $k_1(\varepsilon)$ of Eq. (32.35) has a plateau of the height

$$k_1(\varepsilon) = \frac{\pi}{a} \quad (32.41)$$

at the interval $\sqrt{N} \leq \varepsilon \leq 2\sqrt{N}$. At $\alpha > 1$ we have $k_1 a(\alpha) = \pi\alpha$ in correspondence with (32.34). Thus the lowest root $E_1^{(N)}(\varepsilon)$ of the secular equation (32.32) has the following behaviour as a function of ε :

$$1. \quad E_1^{(N)}(\varepsilon) \simeq \frac{\pi^2 \varepsilon^2}{(2\sqrt{N} - \varepsilon)^2} E_0, \quad 0 < \varepsilon < \sqrt{N}; \quad (32.42a)$$

$$2. \quad E_1^{(N)}(\varepsilon) \simeq \pi^2 E_0, \quad \sqrt{N} < \varepsilon < 2\sqrt{N}; \quad (32.42b)$$

i.e., the curve $E_1^{(N)}$ has a plateau near the energy $E_1 = \pi^2 E_0$ of the first resonance;

$$3. \quad E_1^{(N)}(\varepsilon) \simeq \pi^2 E_0 \left(\frac{\varepsilon}{2\sqrt{N}} \right)^2, \quad \varepsilon > 2\sqrt{N}. \quad (32.42c)$$

These conclusions are in agreement with the result of the direct calculations, presented in Fig. VI.5.

In a similar manner the ε -dependence of the second root $E_2^{(N)}(\varepsilon)$ of the secular equation (32.32) can be analyzed. In this case ($\nu = 2$) the lines

$$y = 2\pi - \frac{ka}{\alpha} \quad (32.43)$$

cross the section OA ($\delta(ka) = -ka$) in the points F_2 with abscissas

$$k_2 a(\varepsilon) = \frac{2\pi\alpha}{(1 - \alpha)}, \quad 0 < \alpha < \frac{1}{3}. \quad (32.44)$$

The crossing points of the type G_2 have constant abscissa

$$k_2 a(\varepsilon) = \pi, \quad \frac{1}{3} < \alpha < \frac{1}{2}. \quad (32.45)$$

It generates the first plateau at the curve $E_2^{(N)}$ near the energy $E_2^{(N)} \simeq \pi^2 E_0$ of the first resonance. This plateau lies in the interval $2\sqrt{N}/3 < \varepsilon < \sqrt{N}$, whose right end coincides with the beginning of the plateau of the curve $E_1^{(N)}$, posed at the same height $\pi^2 E_0$.

The crossing point H_2 of the lines (32.43) with the section BC of the zig-zag line, in which

$$\delta(ka) \simeq \pi - ka \quad (32.46)$$

takes place at the value

$$k_2 a(\alpha) = \frac{\pi\alpha}{1 - \alpha}, \quad \frac{1}{2} < \alpha < \frac{2}{3}, \quad (32.47)$$

i.e., they belong to the same hyperbola (32.40) as the first hyperbolic part of the lowest solution $k_1 a(\varepsilon)$ ($0 < \varepsilon < \frac{1}{2}$). The crossing points K_2 of the lines (32.43) with the section CD of the zig-zag line have constant abscissa

$$k_2 a(\alpha) = 2\pi, \quad \frac{2}{3} < \alpha < 1. \quad (32.48)$$

This fact generates the second plateau at the curve $E_2^{(N)}$ in the interval $4\sqrt{N}/3 < \varepsilon < 2\sqrt{N}$. Its height is close to the energy of the second resonance $E_2 \simeq 4\pi^2 E_0$. At $\varepsilon > 2\sqrt{N}$ we have

$$E_2^{(N)} \simeq 4\pi^2 E_0 \left(\frac{\varepsilon}{2\sqrt{N}} \right)^2. \quad (32.49)$$

It is easy to continue such type of analysis on arbitrary eigenvalues $E_\nu^{(N)}(\varepsilon)$, $\nu \leq N + 1$. The following conclusions can be obtained from this analysis. Each eigenvalue $E_\nu^{(N)}(\varepsilon)$ of the secular equation (32.32) increases monotonically with a growth of ε . Also each solution $k_\nu(\varepsilon)$ of Eq. (32.35) (and corresponding eigenvalue $E_\nu^{(N)}(\varepsilon)$) has plateaux at such values ε_s when $k_\nu(\varepsilon) = \pi s/a$, in other words, when the energy $E_\nu^{(N)}(\varepsilon)$ is close to the position of the s th resonance $E_s \simeq \pi^2 s^2 E_0$, $s = 1, 2, \dots$. Therefore the position of the s th plateau at the various curves $E_\nu^{(N)}(\varepsilon)$ is the same, independently on ν ($s \leq \nu \leq N + 1$). On the value of ν only the total number of plateaux depends. Since in the region $0 < \varepsilon < 2\sqrt{N}$ we have

$0 \leq k_\nu(\varepsilon) \leq \pi\nu/a$, only resonance values $\pi s/a$ with $1 \leq s \leq \nu$ are admissible for $k_\nu(\varepsilon)$. It means that the ν th eigenvalue $E_\nu^{(N)}(\varepsilon)$ as a function of ε has ν plateaux, whose positions are close to the energies $E_s \simeq \pi^2 s^2 E_0$, $s = 1, 2, \dots, \nu$ of ν lowest resonances. The size of plateau decreases when the order number s of the plateau and/or the order number ν of the eigenvalue increases. These conclusions can be illustrated by Fig. VI.6 giving the ε -dependence of the eigenvalue $E_5^{(24)}(\varepsilon)$, obtained by direct diagonalization of the Hamiltonian matrix.

It follows from the previous discussion that the general picture of the set of curves $E_\nu^{(N)}(\varepsilon)$, $\nu = 1, 2, \dots, N+1$ is characterized by the following features:

- 1) At $\varepsilon > 2\sqrt{N}$ we have a set of parabolas

$$E_\nu^{(N)}(\varepsilon) = \pi^2 \nu^2 \left(\frac{\varepsilon}{2\sqrt{N}} \right)^2. \quad (32.50)$$

- 2) In the region $0 < \varepsilon < 2\sqrt{N}$ the curves $E_\nu^{(N)}(\varepsilon)$ form a net constructed from horizontal lines

$$p_\nu = \pi^2 \nu^2 E_0, \quad \nu = 1, 2, \dots, N+1, \quad (32.51)$$

and the curves $h_\nu(\varepsilon)$, described by the equations

$$h_\nu(\varepsilon) = \frac{\pi^2 \nu^2 \varepsilon^2 E_0}{(2\sqrt{N} - \varepsilon)^2}. \quad (32.52)$$

To find the path of the eigenvalue $E_\nu^{(N)}(\varepsilon)$ through this net it is necessary to start from the curve $h_\nu(\varepsilon)$ at $\varepsilon = 0$ and to follow along it up to the crossing point with the horizontal line $p_1 = \pi^2 E_0$. Then it should move along this line up to its crossing point with the curve $h_{\nu-1}(\varepsilon)$. In such a manner the first plateau at the curve $E_\nu^{(N)}(\varepsilon)$ is fixed. Then the movement along $h_{\nu-1}(\varepsilon)$ should be done up to its crossing point with the horizontal $p_2 = 4\pi^2 E_0$, giving the beginning of the second plateau etc.

The results of the numerical calculations, presented in Fig. VI.8, give a good illustration of these semiquantitative predictions. It should be noted that crossing points of the curves $h_\nu(\varepsilon)$ and horizontal lines p_ν are not real contact points of the curve $E_\nu^{(N)}(\varepsilon)$ with the neighbour curves $E_{\nu-1}^{(N)}(\varepsilon)$ or $E_{\nu+1}^{(N)}(\varepsilon)$. Near these points the phenomena of avoiding crossing [16], discussed first by E. Wigner and J.v. Neumann [17], takes place, as it is shown in Fig. VI.9.

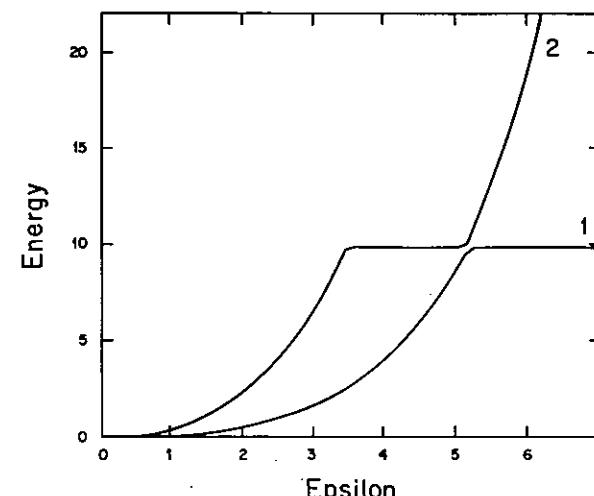
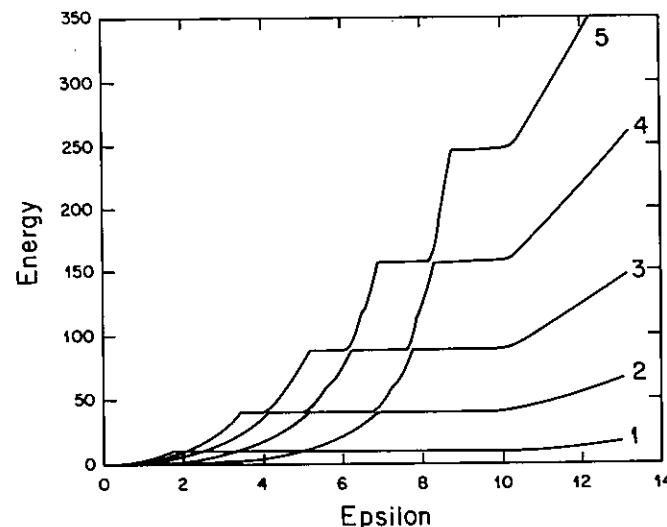


Figure VI.8 (top). The general picture, illustrating the behaviour of few lowest eigenvalues $E_\lambda^{(N)}(\varepsilon)$ ($\lambda = 1, 2, \dots, 5$, $N = 24$, $g = 100$) of the secular equation (32.32) as the functions of the parameter ε .

Figure VI.9 (bottom). The “avoiding of crossing” of two neighbour solutions $E_1^{(N)}(\varepsilon)$ and $E_2^{(N)}(\varepsilon)$ of the secular equation (32.32) for the δ -shell potential ($N = 24$, $g = 100$).

The calculations [16] show also that the slope of each plateau, corresponding to the scattering resonances, grows when the barrier amplitude b decreases and the width Γ of resonance increases.

Although these conclusions were obtained for the concrete potential (32.1) they are valid, at least qualitatively, for arbitrary short range potentials.

Thus, it was shown that the asymptotic approach allows us to understand in a semiquantitative manner how the scattering resonances can be visualized by the analysis of the results of the variational calculations in the harmonic oscillator basis.

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Chapter VII

Group Theory of Harmonic Oscillators

This chapter will deal with the underlying group theory of harmonic oscillators of any dimension and, at the end, with the particular case of the chain of groups $U(3) \supset O(3)$ relevant to the three-dimensional oscillator used in all the previous chapters. Also we will give a condensed presentation of some of the applications of this chain in the $2s-1d$ nuclear shell.

We shall start our discussion with the analysis of the symmetry and dynamical groups underlying the one-dimensional oscillator, as many of the problems we shall face will already appear there, and in a language much more accessible than the one required in higher-dimensional cases.

33 Group Theory of the One-Dimensional Harmonic Oscillator

In the units we have using throughout, *i.e.*, $\hbar = m = \omega = 1$ where m is the mass of the particle and ω the frequency of the oscillator, the Hamiltonian of our problems becomes

$$H = \frac{1}{2}(p^2 + x^2), \quad (33.1)$$

where x, p are a one-dimensional coordinate and momentum. We shall begin by considering x, p, H as classical observables.

We note trivially that this Hamiltonian is invariant under the transformation

$$\begin{pmatrix} \bar{x} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} x \\ p \end{pmatrix}. \quad (33.2a)$$

The set of matrices that appear in (33.2a) form what is known as a group, as the product of two of them has again that form and the same holds for the inverse. This group is known in the literature as O(2) but we note here that it is a rotation in *phase space* and *not* the normal rotation in two-dimensional configuration space (x_1, x_2) .

The matrices in (33.2a) can be changed by a trivial unitary transformation to the form

$$\begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}, \quad (33.2b)$$

and thus the O(2) group is equivalent (isomorphic in the standard language) to U(1), a unitary group in one dimension. In latter discussions the U(1) or O(2) names will be used interchangeably.

We note that the transformation (33.2) is a canonical one as the Poisson brackets of the new coordinate and momentum with respect to the old remain the same [1], *i.e.*,

$$\{\bar{x}, \bar{x}\} = \{\bar{p}, \bar{p}\} = 0, \quad \{\bar{x}, \bar{p}\} = 1. \quad (33.3)$$

Rather than go directly to the discussion of the group of transformation (33.2) we generalize them to arbitrary linear canonical transformations:

$$\begin{pmatrix} \bar{x} \\ \bar{p} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ p \end{pmatrix}, \quad (33.4)$$

where a, b, c, d are real and the determinant of the matrix is 1, *i.e.*,

$$ad - bc = 1. \quad (33.5)$$

It can be immediately seen that this transformation is canonical as (33.3) continues to hold and that it is a group in the sense mentioned above. This group is known in the literature as the two-dimensional real symplectic group $\text{Sp}(2, R)$. A more complete understanding of this group will be given in section 36 when we deal with $\text{Sp}(2n, R)$.

As a, b, c, d are related by (33.5) it is convenient to formulate the matrix in (33.4) in a form that only three of them are independent, and following the well known approach for the rotation group in three dimensions we could write

34. THE LIE ALGEBRA OF LINEAR CANONICAL

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} \cos \chi & \sin \chi \\ -\sin \chi & \cos \chi \end{pmatrix} \begin{pmatrix} e^\theta & 0 \\ 0 & e^{-\theta} \end{pmatrix} \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}, \quad (33.6)$$

in which all the matrices have determinant 1 and

$$0 \leq \chi, \phi \leq 2\pi, \quad -\infty \leq \theta \leq \infty. \quad (33.7)$$

Note that the rotation group in three dimensions has also been put in the (33.6) form but with the replacement θ by $i\theta$ and θ in the interval $0 \leq \theta \leq \pi$. In this case all three parameters χ, θ, ϕ are in a finite range of values and the group is called compact. For $\text{Sp}(2, R)\phi, \chi$ in (33.6) are in the finite interval 0 to 2π , but θ covers all values from $-\infty$ to ∞ . Thus $\text{Sp}(2, R)$ is known as a non compact group. In the following section we shall consider the generators of the corresponding Lie algebra $\text{sp}(2, R)$, *i.e.*, the operators associated with infinitesimal transformations of the type given by (33.4). Note that we shall use capital letters for groups and lower case ones for algebras.

34 The Lie Algebra of Linear Canonical Transformations

To derive the Lie algebra $\text{sp}(2, R)$ we first review the standard procedure through the example of the orthogonal group of two dimensions

$$\bar{x}_1 = x_1 \cos \phi + x_2 \sin \phi, \quad (34.1a)$$

$$\bar{x}_2 = -x_1 \sin \phi + x_2 \cos \phi, \quad (34.1b)$$

which leaves invariant the function $x_1^2 + x_2^2$

If we consider an arbitrary function of these two variables $\psi(x_1, x_2)$ and submit it to an infinitesimal transformation of the type (34.1), *i.e.*,

$$\bar{x}_1 = x_1 + \epsilon x_2, \quad \bar{x}_2 = -\epsilon x_1 + x_2, \quad \epsilon \ll 1, \quad (34.2)$$

we see that the new function $\psi(\bar{x}_1, \bar{x}_2)$, given in terms of the old becomes approximately

$$\psi(x_1 + \epsilon x_2, -\epsilon x_1 + x_2) \simeq \psi(x_1, x_2) - i\epsilon L_3 \psi(x_1, x_2), \quad (34.3)$$

in which L_3 is the operator

$$L_3 = \frac{1}{i} \left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right) = x_1 p_2 - x_2 p_1, \quad (34.4)$$

where on the right hand side we used the *quantum mechanical* definition of momentum in configuration space, *i.e.*,

$$p_1 = \frac{1}{i} \frac{\partial}{\partial x_1}, \quad p_2 = \frac{1}{i} \frac{\partial}{\partial x_2}. \quad (34.5)$$

Note that the operator L_3 is the one for an infinitesimal rotation around the axis x_3 perpendicular to the plane x_1, x_2 .

In our case we have a function of the single configuration space variable, *i.e.*, $\psi(x)$ to which we have to apply a transformation in phase space that can be written in terms of the matrix (33.6). Of the three matrices whose product gives the transformation, the one of dilation is very easy to apply as

$$\bar{x} = e^\theta x \simeq (1 + \epsilon)x, \quad (34.6)$$

where we wrote $\theta = \epsilon$ and assumed $\epsilon \ll 1$. We then have that the effect of dilation is to write $\psi(\bar{x})$ as

$$\psi[(1 + \epsilon)x] = \psi(x) + i\epsilon x \frac{1}{i} \frac{\partial \psi}{\partial x} + \dots = \psi(x) + i\epsilon x \psi' + \dots \quad (34.7)$$

Thus the infinitesimal operator for dilation is xp and, if we want it to be hermitian, we can express it as

$$\frac{1}{2}(xp + px) \equiv 2T_2, \quad (34.8)$$

where we denote the operator as $2T_2$ in the right hand side, as later we want to use the notation T_1, T_2, T_3 for the generators of the $sp(2, R)$ Lie algebra.

There remains though the problem of the calculation of the effect of a rotation in phase space on the function $\psi(x)$. To determine it we go back to section 8 of this book and write again the observables of creation and annihilation of the one-dimensional oscillator in terms of x and p as in (8.2), (8.4), but in the matrix notation

$$\begin{pmatrix} \eta \\ \xi \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \begin{pmatrix} x \\ p \end{pmatrix}. \quad (34.9)$$

The canonical transformation (33.2a) in terms of the new observables becomes

$$\begin{pmatrix} \bar{\eta} \\ \bar{\xi} \end{pmatrix} = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix} \begin{pmatrix} \eta \\ \xi \end{pmatrix}. \quad (34.10)$$

Now we also recall the form (8.1) of the one-dimensional harmonic oscillator states given by the ket $|n\rangle$, where n is the number of quanta, and an arbitrary function $\psi(x)$ can be developed in terms of these kets in the form

$$\psi(x) = \sum_{n=0}^{\infty} a_n |n\rangle = \sum_{n=0}^{\infty} a_n \frac{\eta^n}{\sqrt{n!}} |0\rangle, \quad (34.11)$$

where a_n are appropriate numerical coefficients and $|0\rangle$ is the ground state given in (8.1), while η, ξ will now be considered as operators.

The effect of the form (34.10) of the canonical transformation implies that in (34.11) we replace η by $\bar{\eta} = e^{i\phi}\eta$ and if $\phi = \epsilon$ with $\epsilon \ll 1$ we have $\bar{\eta} \simeq (1 + i\epsilon)\eta$ and $\bar{\eta}^n = (1 + i\epsilon n)\eta^n$. Thus the function $\psi(x)$ of (34.11) is transformed into

$$\sum_{n=0}^{\infty} a_n \frac{(1 + i\epsilon n)\eta^n}{\sqrt{n!}} |0\rangle = (1 + i\epsilon n \xi) \psi, \quad (34.12)$$

where $\eta\xi$ is now the number operator so $\eta\xi|n\rangle = n|n\rangle$ as indicated in (8.6). Thus the generator of the Lie algebra associated with the rotation in phase space of the type (33.2a) is given by the number operator $\eta\xi$ and, as in the case (34.8) for the dilation, we prefer to write it as

$$\frac{1}{2}(\eta\xi + \xi\eta) = \frac{1}{2}(p^2 + x^2) \equiv 2T_3, \quad (34.13)$$

where we made use of the relation (34.9).

If we take the commutator of $2T_2$ and $2T_3$ we get the operator

$$[2T_2, 2T_3] = -i(\eta^2 + \xi^2) = i(p^2 - x^2) \equiv 4iT_1. \quad (34.14)$$

We thus have, both in the notation (x, p) with p of the form (34.5), and (η, ξ) , the form of the operator T_1, T_2, T_3 that satisfy the commutation rules

$$[T_1, T_2] = -iT_3, [T_2, T_3] = iT_1, [T_3, T_1] = iT_2, \quad (34.15)$$

which correspond to those of the $sp(2, R)$ Lie algebra or to the isomorphic one $su(1, 1)$.

Note that all operators $T_i, i = 1, 2, 3$ are Hermitian and that the commutator rules are similar to those of $L_i, i = 1, 2, 3$ of the rotation group, except for the first commutation rule in (34.15) that has the opposite sign. This slight change make all the difference between the compact group $O(3)$ and the noncompact one $Sp(2, R)$.

The generator T_3 in (34.13) is the one associated with the canonical transformations (33.2a) that leave invariant the Hamiltonian (33.1) of the one-dimensional oscillator, and thus it is the single generator of the Lie algebra of the rotation group $O(2)$ in (33.2a) or, if we speak in the language of η, ξ , of the unitary group $U(1)$ corresponding to the transformation $\bar{\eta} = \eta e^{i\phi}$ in (33.10), as $\bar{\xi} = \xi e^{-i\phi}$ is obtained from the former by Hermitian conjugation.

If we dealt with the ordinary rotation group (34.2) in the two-dimensional configuration space the single generator is the L_3 of (34.4) and the basis for the irreducible representation [2] (BIR) are the function $\exp(im\phi)$, with $\phi = \arctan(x_2/x_1)$ which are eigenstates of L_3 with eigenvalue m . For the rotation in phase space given by (33.2a) the generator of the Lie algebra is T_3 of (34.13) and, as it is proportional to the Hamiltonian of the one-dimensional oscillator (33.1), it is clear that its BIR are the eigenkets $|n\rangle$ of (8.1) for which

$$T_3|n\rangle = \frac{1}{2}(n + \frac{1}{2})|n\rangle. \quad (34.16)$$

Thus the number of quanta n of the states of the one-dimensional harmonic oscillator characterize the BIR of the group $U(1)$, or equivalently, $O(2)$, of which T_3 is the generator.

For the full group $Sp(2, R)$ the BIR are characterized by the eigenvalues of the Casimir operator of this group [3], which is defined as the one that commutes with all the generators T_i , $i = 1, 2, 3$ and, from (34.15) we can show that it has this property when it is given by

$$T^2 \equiv T_1^2 + T_2^2 - T_3^2. \quad (34.17)$$

The operator T^2 plays for $Sp(2, R)$ the role that $L^2 = L_1^2 + L_2^2 + L_3^2$ plays for $O(3)$, in the sense that the BIR of both groups are given respectively by the eigenstates of T^2 and L^2 .

We shall proceed to prove that all the even states of the harmonic oscillator $|2n\rangle$, $n = 0, 1, 2, \dots$ and all the odd ones $|2n+1\rangle$, $n = 0, 1, \dots$, correspond to definite eigenvalues of T^2 , and so they are BIR of the $Sp(2, R)$ group.

To achieve this purpose we note that from (34.8,13,14) we have

$$T_1 = -\frac{1}{4}(\eta^2 + \xi^2), T_2 = \frac{i}{4}(\eta^2 - \xi^2), T_3 = \frac{1}{4}(\eta\xi + \xi\eta) = \frac{1}{2}(\eta\xi + \frac{1}{2}), \quad (34.18)$$

which imply that

$$T_+ \equiv T_1 + iT_2 = -\frac{1}{2}\eta^2, T_- \equiv T_1 - iT_2 = -\frac{1}{2}\xi^2, [T_-, T_+] = 2T_3, \quad (34.19)$$

also commute with T^2 of (34.17), and that the latter can be written as

$$T^2 = T_+T_- - T_3(T_3 - 1). \quad (34.20)$$

From (8.1), (34.19) we see that all states $|2n\rangle$ can be obtained from T_+^n applied to the ground state $|0\rangle$, while all states $|2n+1\rangle$ can come from

applying the same operator to the first excited state $|1\rangle$. As T_+^n commutes with T^2 it is clear that when applying T^2 to $|2n\rangle$ or $|2n+1\rangle$ we get the same results as when we apply them to $|0\rangle$ or $|1\rangle$. Furthermore, from (34.19) we see that

$$T_-|0\rangle = T_-|1\rangle = 0, \quad (34.21)$$

so that

$$T^2|0\rangle = -T_3(T_3 - 1)|0\rangle = \frac{3}{16}|0\rangle, \quad (34.22)$$

$$T^2|1\rangle = -T_3(T_3 - 1)|1\rangle = \frac{3}{16}|1\rangle, \quad (34.23)$$

thus proving that all even states $|2n\rangle$, $n = 0, 1, 2, \dots$, correspond to the BIR of $Sp(2, R)$ characterized by the eigenvalue $-t(t-1) = \frac{3}{16}$ of T^2 where $t = \frac{1}{4}$ and which we could denote as the even irreducible representation, while all the states $|2n+1\rangle$, $n = 0, 1, 2, \dots$, form part of an odd irreducible representation characterized by the eigenvalue $t = 3/4$. These irreducible representations are ∞ dimensional as required by the noncompact character of the group.

The characterization of *all* the states $|n\rangle$, $n = 0, 1, 2, \dots$ by BIR of the $Sp(2, R)$, with the single eigenvalue $3/16$ of T^2 , is responsible for the fact that $Sp(2, R)$ receives the name of dynamical group, while $U(1)$ whose generator is T_3 is called the symmetry group.

35 The Representation in Quantum Mechanics of the Group of Linear Canonical Transformations

If we have the group of linear canonical transformation (33.4) in classical phase space, we would like to know what is its effect in quantum mechanics on a wave function $\psi(x)$ which, in the bracket notation of Dirac, we denote as

$$\psi(x') \equiv \langle x'|\psi\rangle. \quad (35.1)$$

In this section we shall also adopt Dirac [4] notation in the sense that x, p will be quantum mechanical operators while primed expressions such as x', x'' will correspond to ordinary variables.

According to Dirac [5], if we have a canonical transformation such as the one in (33.4), which is bijective, *i.e.*, one to one, and where the initial

and final variables have spectra going from $-\infty$ to ∞ , the corresponding relation between \bar{x}, \bar{p} and x, p is

$$\bar{x} = \mathcal{U}x \mathcal{U}^{-1}, \quad (35.2a)$$

$$\bar{p} = \mathcal{U}p \mathcal{U}^{-1}, \quad (35.2b)$$

where the operator \mathcal{U} is unitary, i.e., $\mathcal{U}^{-1} = \mathcal{U}^\dagger$.

Our objective will be to determine \mathcal{U} in the configuration space representation, i.e.,

$$\langle x' | \mathcal{U} | x'' \rangle, \quad (35.3)$$

which allows to consider the effect of any canonical transformation (33.4) on an arbitrary function $\psi(x')$, i.e.,

$$\langle x' | \bar{\psi} \rangle = \int_{-\infty}^{\infty} \langle x' | \mathcal{U} | x'' \rangle dx'' \langle x'' | \psi \rangle. \quad (35.4)$$

To achieve our objective we first note that the representation of the operators of coordinate x and momenta p in the configuration space basis is [6]

$$\langle x' | x | x'' \rangle = x' \delta(x' - x''), \quad (35.5)$$

$$\langle x' | p | x'' \rangle = \frac{1}{i} \frac{\partial}{\partial x'} \delta(x' - x'') = -\frac{1}{i} \frac{\partial}{\partial x''} \delta(x' - x''). \quad (35.6)$$

Equations (35.2) can also be written as

$$\bar{x}\mathcal{U} = \mathcal{U}x, \quad (35.7a)$$

$$\bar{p}\mathcal{U} = \mathcal{U}p, \quad (35.7b)$$

and if we take their matrices between a bra $\langle x' |$ and a ket $| x'' \rangle$ we obtain

$$\begin{aligned} & \int_{-\infty}^{\infty} \langle x' | \bar{x} | x''' \rangle dx''' \langle x''' | \mathcal{U} | x'' \rangle \\ &= \int_{-\infty}^{\infty} \langle x' | \mathcal{U} | x''' \rangle dx''' \langle x''' | x | x'' \rangle, \end{aligned} \quad (35.8a)$$

$$\begin{aligned} & \int_{-\infty}^{\infty} \langle x' | \bar{p} | x''' \rangle dx''' \langle x''' | \mathcal{U} | x'' \rangle \\ &= \int_{-\infty}^{\infty} \langle x' | \mathcal{U} | x''' \rangle dx''' \langle x''' | p | x'' \rangle, \end{aligned} \quad (35.8b)$$

where we introduced intermediate kets and bras in x''' as is usually done in matrix or operator products.

If we now replace \bar{x}, \bar{p} by their values in (33.4) and consider the resulting x, p in their operator form (35.5), (35.6), we note that $\langle x' | \mathcal{U} | x'' \rangle$ satisfies the following two partial differential equations:

$$(ax' + \frac{b}{i} \frac{\partial}{\partial x'}) \langle x' | \mathcal{U} | x'' \rangle = x'' \langle x' | \mathcal{U} | x'' \rangle, \quad (35.9a)$$

$$(cx' + \frac{d}{i} \frac{\partial}{\partial x'}) \langle x' | \mathcal{U} | x'' \rangle = -\frac{1}{i} \frac{\partial}{\partial x''} \langle x' | \mathcal{U} | x'' \rangle. \quad (35.9b)$$

The term on the right hand side of (35.9b) comes from the fact that for $\langle x''' | p | x'' \rangle$ we take the form at the end of Eq. (35.6), i.e., $-(1/i)\partial/\partial x'' \delta(x''' - x'')$. Thus we can take $-(1/i)\partial/\partial x''$ outside the integral in x''' in the right hand side of (35.9b) and carrying the integration with $\delta(x''' - x'')$ we obtain the last term in (35.9b).

Equations (35.9) were first derived by Moshinsky and Quesne [7] and, for more general canonical transformations, by Mello and Moshinsky [8]. For short they will be called the M. M. equations from the initials of the authors of the last paper, though colloquially in Mexico they are known as the Marilyn Monroe equations, where the initials are the same but the sex appeal is much greater.

A solution of (35.9) that suggests itself, is an exponential of a bilinear expression in x', x'' as its derivatives give factors that are linear in these variables. Thus we propose that

$$\langle x' | \mathcal{U} | x'' \rangle = A \exp [i(\lambda x'^2 + \mu x' x'' + \nu x''^2)], \quad (35.10)$$

where λ, μ, ν are constants yet to be determined and A will be evaluated through a normalization condition.

Substituting (35.10) in the two equation (35.9), and eliminating the exponential term that appears everywhere, we get the following equations:

$$(a + 2\lambda b)x' + (\mu b - 1)x'' = 0, \quad (35.11a)$$

$$(c + 2\lambda d + \mu)x' + (d\mu + 2\nu)x'' = 0. \quad (35.11b)$$

As x', x'' are arbitrary, the four coefficients must vanish, which leads to values of λ, μ, ν given by

$$\lambda = -(a/2b), \quad (35.12a)$$

$$\mu = (1/b), \quad (35.12b)$$

$$\nu = -(d/2b), \quad (35.12c)$$

together with the condition $ad - bc = 1$, which was already required in (33.4) if we wanted to have a canonical transformation.

For the coefficient A we draw on the fact that \mathcal{U} is unitary so $\mathcal{U}^{-1} = \mathcal{U}^\dagger$ and thus

$$\langle x' | \mathcal{U} \mathcal{U}^\dagger | x'' \rangle = \delta(x' - x''). \quad (35.13)$$

Writing it out explicitly we obtain

$$\begin{aligned} \int_{-\infty}^{\infty} \langle x' | \mathcal{U} | x''' \rangle dx''' \langle x''' | \mathcal{U}^\dagger | x'' \rangle = \\ \int_{-\infty}^{\infty} \langle x' | \mathcal{U} | x''' \rangle \langle x'' | \mathcal{U} | x''' \rangle^* dx''' = \delta(x' - x''). \end{aligned} \quad (35.14)$$

If in the last integral in (35.14) we substitute $\langle x' | \mathcal{U} | x'' \rangle$ by its expression (35.10), where λ, μ, ν have the values (35.12), we obtain for (35.14) the value

$$2\pi|A|^2 b \delta(x' - x''), \quad (35.15)$$

so, assuming A real, the unitary character holds if $A = (2\pi b)^{-1/2}$ and we can write the unitary operator in the configuration space representation as [9]

$$\langle x' | \mathcal{U} | x'' \rangle = (2\pi b)^{-1/2} \exp [(-i/2b)(ax'^2 - 2x'x'' + dx''^2)]. \quad (35.16)$$

Clearly the above representation is valid only for canonical transformations where $b \neq 0$. If $b = 0$ the simplest way to make the analysis is to consider the development for arbitrary canonical transformations given by (33.6). For the dilation associated with e^θ the unitary representation is clearly $\delta(x'' - e^\theta x')$, while for rotation in phase space it is given by (35.16) when $a = d = \cos \phi$ and $b = -c = \sin \phi$. Thus carrying out in the standard way the product for the unitary representations of the three factors in (33.6), we can obtain the appropriate expression even if $b = 0$.

Once we have the representation in configuration space of the unitary operator associated with a canonical transformation, we can pass to any other basis. For example, if we want to consider the representation in the basis of harmonic oscillator states, it is given by double integral

$$\langle n' | \mathcal{U} | n'' \rangle = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \langle n' | x' \rangle dx' \langle x' | \mathcal{U} | x'' \rangle dx'' \langle x'' | n'' \rangle, \quad (35.17)$$

where $\langle x'' | n'' \rangle$ is the state of the one-dimensional oscillator of (8.1) where now x is replaced by x'' and n by n'' , and similarly for $\langle n' | x' \rangle = \langle x' | n' \rangle^*$. An explicit derivation of $\langle n' | \mathcal{U} | n'' \rangle$, using the generating functions of the harmonic oscillator states, was given by Moshinsky and Quesne [9].

We have thus completed the discussion of the symmetry and dynamical Lie algebras of the one-dimensional oscillator and their representation in quantum mechanics.

36 Group Theory of the n -Dimensional Harmonic Oscillator

We now have the classical coordinates x_i , and momenta p_i with an index $i = 1, 2, \dots, n$. In the units mentioned at the beginning of section 33 the Hamiltonian becomes

$$H = \frac{1}{2} \sum_{i=1}^n (p_i^2 + x_i^2) = \sum_{i=1}^n (\eta_i \xi_i) + (n/2), \quad (36.1)$$

where we have used the definition (8.4) or (34.9) for η_i, ξ_i , just adding the index i .

To see what is the symmetry group of this Hamiltonian we look at its form on the right hand side (r.h.s.) of (36.1) and consider the transformation

$$\bar{\eta}_i = \sum_{j=1}^n U_{ij} \eta_j, \quad (36.2a)$$

where $U = \|U_{ij}\|$ is a unitary matrix. As classically $\xi_i = \eta_i^*$, taking the complex conjugate of (36.2a) we obtain

$$\bar{\xi}_i = \sum_{j=1}^n U_{ij}^* \xi_j = \sum_{j=1}^n \xi_j U_{ji}^*. \quad (36.2b)$$

From the unitary character of U we have that

$$\sum_{i=1}^n U_{ij} U_{ik}^* = \sum_{i=1}^n U_{ki}^* U_{ij} = \delta_{kj}, \quad (36.3)$$

so that we obtain

$$\sum_{i=1}^n \bar{\eta}_i \bar{\xi}_i = \sum_{i=1}^n \eta_i \xi_i, \quad (36.4)$$

and the Hamiltonian (36.1), in the form of the r.h.s. of (36.1), remains invariant under a unitary transformation of the type indicated in (36.2).

The Poisson brackets of $\bar{\eta}_i, \bar{\xi}_j$ are clearly the same as those of η_i, ξ_j as

$$\{\bar{\eta}_i, \bar{\eta}_j\} = 0 \quad (36.5a)$$

$$\{\bar{\xi}_i, \bar{\xi}_j\} = 0, \quad (36.5b)$$

because $\{\eta_i, \eta_j\} = 0$ and so do the $\{\xi_i, \xi_j\} = 0$ while

$$\{\bar{\xi}_i, \bar{\eta}_j\} = \left\{ \sum_k U_{ik}^* \xi_k, \sum_\ell U_{j\ell} \eta_\ell \right\} = -i \sum_k U_{ik}^* U_{jk} = -i \delta_{ij}, \quad (36.5c)$$

using the fact that $\{\xi_k, \eta_\ell\} = -i\delta_{k\ell}$. We note also that from the relations between \bar{x}_i, \bar{p}_i and $\bar{\eta}_i, \bar{\xi}_i$, we have for the former the Poisson brackets

$$\{\bar{x}_i, \bar{x}_j\} = 0, \quad (36.5d)$$

$$\{\bar{p}_i, \bar{p}_j\} = 0, \quad (36.5e)$$

$$\{\bar{x}_i, \bar{p}_j\} = \delta_{ij}, \quad (36.5f)$$

which are the same as those of x_i, p_i and thus we are dealing with a canonical transformation.

What is the form of the unitary transformation (36.2) in the phase space, i.e., in $x_i, p_i, i = 1, 2, \dots, n$? To determine it we introduce column vector notation in bold face letters:

$$\boldsymbol{\eta}, \boldsymbol{\xi}, \mathbf{x}, \mathbf{p}, \quad (36.6)$$

whose components are given by the same letter with index $i = 1, 2, \dots, n$. The transformation (36.2) can then be written as

$$\begin{pmatrix} \bar{\eta} \\ \bar{\xi} \end{pmatrix} = \begin{pmatrix} \mathbf{U} & 0 \\ 0 & \mathbf{U}^* \end{pmatrix} \begin{pmatrix} \eta \\ \xi \end{pmatrix}, \quad (36.7)$$

and to pass to phase space we can use (34.9) where everything is bold face and $1, i$ are replaced by $\mathbf{I}, i\mathbf{I}$ with \mathbf{I} being the unit $n \times n$ matrix. We arrive then immediately at the relation

$$\begin{bmatrix} \bar{\mathbf{x}} \\ \bar{\mathbf{p}} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} (\mathbf{U} + \mathbf{U}^*) & -i(\mathbf{U} - \mathbf{U}^*) \\ i(\mathbf{U} - \mathbf{U}^*) & (\mathbf{U} + \mathbf{U}^*) \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ \mathbf{p} \end{bmatrix}, \quad (36.8)$$

which is clearly a real and, from the discussion in (36.5), also a canonical transformation.

As in the case of the one-dimensional oscillator in section 33, it is convenient to generalize (36.8) to arbitrary linear canonical transformations, before proceeding, as we did in section 35, to determine their unitary representation in quantum mechanics. For this purpose it is convenient to represent classical coordinates and momenta $x_i, p_i, i = 1, 2, \dots, n$ by a single letter $z_\alpha, \alpha = 1, 2, \dots, 2n$, that are components of a $2n$ -dimensional vector in the phase space defined by

$$z_i \equiv x_i, \quad (36.9a)$$

$$z_{i+n} \equiv p_i. \quad (36.9b)$$

The Poisson bracket of two observables f, g is then given by

$$\{f, g\} = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial x_i} \right) = \sum_{\alpha, \beta=1}^{2n} \frac{\partial f}{\partial z_\alpha} K_{\alpha\beta} \frac{\partial g}{\partial z_\beta}, \quad (36.10)$$

where the matrix is

$$\mathbf{K} = \|K_{\alpha\beta}\| = \begin{pmatrix} 0 & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}, \quad (36.11)$$

with all submatrices being of dimension $n \times n$.

If we now pass from a vector $\{z_\alpha\}$ in phase space to another one $\{\bar{z}_\alpha\}$, whose components are functions of the previous one, the transformation will be canonical when [10]

$$\sum_{\gamma, \delta} \frac{\partial \bar{z}_\alpha}{\partial z_\gamma} K_{\gamma\delta} \frac{\partial \bar{z}_\beta}{\partial z_\delta} = K_{\alpha\beta}. \quad (36.12)$$

If, in particular, the transformation between the new and old vectors in phase space is linear, i.e.,

$$\bar{z}_\alpha = \sum_\beta S_{\alpha\beta} z_\beta, \quad (36.13)$$

the transformation will be canonical if

$$\mathbf{SK}\tilde{\mathbf{S}} = \mathbf{K}, \quad (36.14)$$

where $\mathbf{S} = \|S_{\alpha\beta}\|$ and the tilde stands for transposed. The matrix \mathbf{S} will be assumed real so that \bar{x}_i and \bar{p}_i remain Hermitian when later x_i and p_i are represented by Hermitian operators in quantum mechanics.

The matrix \mathbf{K} is the one usually associated with the symplectic group. Thus the matrices \mathbf{S} satisfying (36.14) are elements of an $2n$ -dimensional real symplectic group $\text{Sp}(2n, R)$. We shall write these matrices in the form

$$\mathbf{S} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix}, \quad (36.15)$$

where the real submatrices are all of dimension $n \times n$ with components

$$\mathbf{A} = \|a_{ij}\|, \quad \mathbf{B} = \|b_{ij}\|, \quad \mathbf{C} = \|c_{ij}\|, \quad \mathbf{D} = \|d_{ij}\|. \quad (36.16)$$

The restrictions (36.14) lead then to the equations

$$\mathbf{B}\tilde{\mathbf{A}} = \mathbf{A}\tilde{\mathbf{B}}, \quad (36.17a)$$

$$\mathbf{C}\tilde{\mathbf{D}} = \mathbf{D}\tilde{\mathbf{C}}, \quad (36.17b)$$

$$(\mathbf{D}\tilde{\mathbf{A}} - \mathbf{C}\tilde{\mathbf{B}}) = \mathbf{I}, \quad (36.17c)$$

and it is easy to see that if $\mathbf{A} = \mathbf{D} = (1/2)(\mathbf{U} + \mathbf{U}^*)$, $-\mathbf{B} = \mathbf{C} = (i/2)(\mathbf{U} - \mathbf{U}^*)$, they satisfy these conditions if we make use of the fact that \mathbf{U} is unitary, i.e., $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}\tilde{\mathbf{U}}^* = \mathbf{I}$.

In section 35 we found it convenient to discuss first the case $b \neq 0$, and here we shall start with the equivalent supposition that

$$\det \mathbf{B} \neq 0, \quad (36.18)$$

which implies that \mathbf{B}^{-1} exists and from (36.17c) we could write

$$\mathbf{C} = (\mathbf{D}\tilde{\mathbf{A}} - \mathbf{I})\tilde{\mathbf{B}}^{-1}. \quad (36.19)$$

From this equation and (36.17a,b) we see that the restrictions on the remaining submatrices \mathbf{A} , \mathbf{B} and \mathbf{D} are given by

$$\mathbf{B}\tilde{\mathbf{A}} = \mathbf{A}\tilde{\mathbf{B}}, \quad (36.20a)$$

$$\tilde{\mathbf{B}}\mathbf{D} = \tilde{\mathbf{D}}\mathbf{B}. \quad (36.20b)$$

Equations (36.20) are the ones that determine the general matrix \mathbf{S} when $\det \mathbf{B} \neq 0$.

We turn now to the question of what is the unitary representation in the configuration space of quantum mechanics of the linear symplectic transformation (36.15), when $\det \mathbf{B} \neq 0$ and the condition (36.20) are satisfied. The analysis follows a procedure very similar to the one described in section 35 for the symplectic transformation (33.4) when $b \neq 0$, so we just give the result for the unitary representation [7]

$$\begin{aligned} \langle \mathbf{x}' | \mathcal{U} | \mathbf{x}'' \rangle &= [(2\pi)^n |\det \mathbf{B}|]^{-\frac{1}{2}} \\ &\times \exp \left[-\left(\frac{i}{2}\right) (\tilde{\mathbf{x}}' \mathbf{B}^{-1} \mathbf{A} \mathbf{x}' - 2\tilde{\mathbf{x}}' \mathbf{B}^{-1} \mathbf{x}'' + \tilde{\mathbf{x}}'' \mathbf{D} \mathbf{B}^{-1} \mathbf{x}'') \right], \end{aligned} \quad (36.21)$$

which is very similar to the one corresponding to the two-dimensional phase space given by (35.16). For the case when $\det \mathbf{B} = 0$ the analysis is somewhat different and the result is derived in reference [7].

Thus we conclude that we have both a dynamical Lie group $\text{Sp}(2n, R)$ and symmetry Lie group $\text{U}(n)$ for the n -dimensional oscillator. We also give the unitary representation in quantum mechanics of $\text{Sp}(2n, R)$ which includes of course that of $\text{U}(n)$ when $\mathbf{A} = \mathbf{D} = (1/2)(\mathbf{U} + \mathbf{U}^*)$, $-\mathbf{B} = \mathbf{C} = (i/2)(\mathbf{U} - \mathbf{U}^*)$.

37 Lie Algebra for Systems of m Oscillators in n Dimensions

We shall now carry all the discussion in quantum mechanics so our coordinate and momenta operators will be denoted by

$$x_{is}, p_{is}, \quad i = 1, 2, \dots n; \quad s = 1, 2, \dots m, \quad (37.1)$$

and the corresponding creation and annihilation operators, related to them through (8.4) or (34.9), are

$$\eta_{is}, \xi_{is}. \quad (37.2)$$

The Hamiltonian operator for our oscillator problem can be written as

$$\begin{aligned} H &= \frac{1}{2} \sum_{s=1}^m \sum_{i=1}^n (p_{is}^2 + x_{is}^2) = \frac{1}{2} \sum_{s=1}^m \sum_{i=1}^n (\eta_{is} \xi_{is} + \xi_{is} \eta_{is}) \\ &= \sum_{s=1}^m \sum_{i=1}^n (\eta_{is} \xi_{is}) + \frac{mn}{2}. \end{aligned} \quad (37.3)$$

With the experience of the previous sections and, in particular, of Eqs. (34.18) and (34.19) we expect that the symplectic Lie algebra of mn dimensions, i.e., $\text{sp}(2mn, R)$ that we can associate with it would be the $mn(2mn + 1)$ bilinear expressions in the operators (37.2), i.e.,

$$\eta_{is} \eta_{jt}, \quad (37.4a)$$

$$(1/2)(\eta_{is} \xi_{jt} + \xi_{jt} \eta_{is}), \quad (37.4b)$$

$$\xi_{is} \xi_{jt}, \quad (37.4c)$$

where j, t have the same range of values (37.1) as i, s .

The Poisson brackets are now replaced by commutators and as we have

$$[\eta_{is}, \eta_{jt}] = 0, \quad (37.5a)$$

$$[\xi_{is}, \xi_{jt}] = 0, \quad (37.5b)$$

$$[\xi_{is}, \eta_{jt}] = \delta_{ij} \delta_{st}, \quad (37.5c)$$

it is clear that *the commutator of any pair of terms in (37.4) gives a linear combination of elements of this type*, which is the property that characterizes a Lie algebra. The fact that the operators correspond to infinitesimal transformations of the group $\text{Sp}(2mn, R)$ could be proved by a procedure similar to the one we carried out for $\text{Sp}(2, R)$ in section 34.

As in Eq. (8.16) for the case of one particle in an oscillator of three dimensions, the eigenstates of the Hamiltonian (37.3) can be expressed by homogeneous polynomials of degree N in η_{is} acting on the ground state:

$$|0\rangle = \pi^{-(mn/4)} \exp \left[-(1/2) \sum_{s=1}^m \sum_{i=1}^n x_{is}^2 \right], \quad (37.6)$$

and the corresponding eigenvalue of H will be

$$N + \frac{mn}{2}, \quad (37.7)$$

where N will be denoted as the number of quanta.

By applying the elements $\xi_{is}\xi_{jt}$ of the Lie algebra $\text{sp}(2mn, R)$ to the state of N quanta we can change it to one with $N - 2$ quanta and thus following the procedure we can reduce all states either to the ground state $|0\rangle$ or to the one-quantum state:

$$|1, is\rangle \equiv \eta_{is}|0\rangle, \quad i = 1, 2, \dots, n; \quad s = 1, 2, \dots, m, \quad (37.8)$$

using only elements of the Lie algebra. Thus, as for the one-dimensional oscillator, all states of even number quanta belong to one infinite-dimensional unitary irreducible representation of $\text{Sp}(2mn, R)$ while all odd ones belong to another.

Of more interest is the situation for the symmetry Lie algebra formed from all the generators (37.4b) which, from (37.3), commute with H . We get rid of constant numerical terms and write these $(nm)^2$ generators as

$$\mathcal{C}_{is,jt} \equiv \eta_{is}\xi_{jt}, \quad (37.9)$$

where from (37.5) we have the commutation relations

$$[\mathcal{C}_{is,jt}, \mathcal{C}_{i's',j't'}] = \mathcal{C}_{is,jt'}\delta_{i'j}\delta_{s't} - \mathcal{C}_{i's',jt}\delta_{ij}\delta_{st'}, \quad (37.10)$$

which identifies them [11] as members of a unitary Lie algebra of nm dimensions, which is the symmetry Lie algebra of the Hamiltonian (37.3) and corresponds to the group $\text{U}(mn)$.

In this section we shall be mainly interested in two subalgebras of $\text{U}(mn)$ of which extensive use will be made in the following section. One of them is related to the fact that if we take $s = t$ in (37.9), and fix this number, we have generators of the form

$$\mathcal{C}_{ij}(s) = \eta_{is}\xi_{js}, \quad (37.11)$$

which correspond to a unitary group in n dimensions $\text{U}(n)$, as the commutation rules are

$$[\mathcal{C}_{ij}(s), \mathcal{C}_{i'j'}(s)] = \mathcal{C}_{ij'}(s)\delta_{i'j} - \mathcal{C}_{i'j}(s)\delta_{ij'}, \quad (37.12)$$

while $\mathcal{C}_{ij}(s)$ and $\mathcal{C}_{i'j'}(t)$ with $s \neq t$, commute. This then leads to the chain of algebras

$$\text{u}(mn) \supset \text{u}_1(n) \oplus \text{u}_2(n) \dots \oplus \text{u}_m(n), \quad (37.13)$$

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where the symbol \oplus indicates a direct sum.

The Lie algebra of other subgroups can be formed when we contract $\mathcal{C}_{is,jt}$ either with respect to the oscillator number or the dimension number, *i.e.*,

$$\mathcal{C}_{ij} = \sum_{s=1}^m \mathcal{C}_{is,js}, \quad (37.14a)$$

$$\mathcal{C}_{st} = \sum_{i=1}^n \mathcal{C}_{is,ii}, \quad (37.14b)$$

where the \mathcal{C}_{ij} have the same commutation rules as (37.11) but with the s parameter suppressed and a similar result holds for the \mathcal{C}_{st} . Thus in this case we have the chain of groups

$$\text{U}(mn) \supset \text{U}(n) \otimes \text{U}(m), \quad (37.15)$$

where the symbol \otimes indicates a direct product. The \mathcal{C}_{ij} are the generators of $\text{U}(n)$ and \mathcal{C}_{st} those of $\text{U}(m)$, and using (37.10) it can be immediately proved that

$$[\mathcal{C}_{ij}, \mathcal{C}_{st}] = 0. \quad (37.16)$$

Finally, in connection with the unitary groups, we would like to speak of their Casimir operators, *i.e.*, functions of the generators that commute with all the generators as for example L^2 commutes with L_i , $i = 1, 2, 3$, in the case of the three-dimensional orthogonal groups $O(3)$.

We shall take as an example the \mathcal{C}_{ij} of $\text{U}(n)$ in (37.14a). It is easy to see with the help of (37.12) (in which we suppress the s) that the trace of arbitrary powers of the matrix $\mathcal{C} = \|\mathcal{C}_{ij}\|$ commutes with all \mathcal{C}_{ij} . Thus,

$$\Gamma_1 = \sum_{i=1}^n \mathcal{C}_{ii}, \quad (37.17a)$$

$$\Gamma_2 = \sum_{i,j=1}^n \mathcal{C}_{ij}\mathcal{C}_{ji}, \quad (37.17b)$$

$$\Gamma_3 = \sum_{i,j,k=1}^n \mathcal{C}_{ij}\mathcal{C}_{jk}\mathcal{C}_{ki}, \quad (37.17c)$$

and so on, are Casimir operators of $\text{U}(n)$.

It may happen though that, after a certain power, the Γ 's become functionally dependent on the previous ones, and thus they provide no further

information. The irreducible representations of $U(n)$ are characterized unambiguously by the eigenvalues of the first n Casimir operators [11].

The same holds for C_{st} of $U(m)$ where, by a similar reasoning, we see that the trace of the matrix $\mathbf{C} = \|C_{st}\|$ commutes with all C_{st} . Thus,

$$\Delta_1 = \sum_{s=1}^m C_{ss}, \quad (37.18a)$$

$$\Delta_2 = \sum_{s,t=1}^m C_{st} C_{ts}, \quad (37.18b)$$

$$\Delta_3 = \sum_{s,t,u=1}^m C_{st} C_{tu} C_{us}, \quad (37.18c)$$

and so on, are Casimir operators of $U(m)$.

The interesting point is that the Γ 's and Δ 's are related as can be seen by writing C_{ij} and C_{st} explicitly in η_{is} and ξ_{ji} . In fact we have

$$\Gamma_1 = \Delta_1, \quad (37.19a)$$

$$\Gamma_2 = \Delta_2 + (n-m)\Delta_1, \quad (37.19b)$$

$$\Gamma_3 = \Delta_3 + 2(n-m)\Delta_2 + (n-m)^2\Delta_1, \quad (37.19c)$$

and so on, so that the groups $U(n)$ and $U(m)$ are complementary [12], in the sense that if the irreducible representation of $U(n)$ is fixed by the eigenvalues of the Casimir operators $\Gamma_s, s = 1, \dots, n$, then so are those of $U(m)$ by the eigenvalues of $\Delta_s, s = 1, \dots, m$, related to the previous ones as in (37.19), a fact of which use will be made in the following sections.

38 The Group $U(3)$ for Systems of 1 and 2 Particles, As Well As for 3, But Only in Relative Motion

In chapters 1 to 6 of this book no group theory was used, (except for permutations of 3 or 4 particles) and only the many particle states in a three-dimensional harmonic oscillator were employed in all the developments. We showed though, in the previous sections, that these states are actually related with the irreducible representations of groups and, in particular, with those of the $U(3n)$ group where n is the number of particles.

In this section we review some of our previous states in group theoretical language, following the chain of (37.13) for the Lie algebras, *i.e.*,

$$u(3n) \supset u_1(3) \oplus u_2(3) \dots \oplus u_n(3). \quad (38.1)$$

In all of these states we are interested in definite angular momenta for the particles so for the $u(3)$ Lie algebras in (38.1) we will be concerned with the chain

$$u(3) \supset o(3) \supset o(2), \quad (38.2)$$

where the o corresponds to an orthogonal Lie algebras of the dimension indicated.

We shall also discuss new type of states related with the chain of groups (37.15), *i.e.*,

$$U(3n) \supset U(3) \otimes U(n), \quad (38.3)$$

where again we will be interested in states of definite angular momentum, so for $U(3)$ we shall consider the same chain of subgroups as for the Lie algebra $u(3)$ in (38.2). These new states were shown by Elliott [13,14] to be very relevant for collective effects in nuclei and so it is important to discuss them in a book on the harmonic oscillator, and they could also be of interest in the structure of baryons as formed from three quarks.

a) States for the chain (38.1)

We start with the one particle problem, *i.e.*, when $n = 1$. In that case for the chain (38.2) the states are clearly those discussed in section 8 of this book, as the Casimir operator of $u(3)$, *i.e.*, Γ_1 of (37.17a) is clearly the number operator

$$\Gamma_1 \equiv \hat{N} = \boldsymbol{\eta} \cdot \boldsymbol{\xi}, \quad (38.4)$$

while the corresponding ones to $o(3)$ and $o(2)$ are L^2 and L_3 with L given in terms of the creation and annihilation operators by (8.15).

The states for the chain (38.2) of Lie algebras are then polynomials in the creation operators $\eta_i, i = 1, 2, 3$ acting on the ground state and given by the ket $|nlm\rangle$ of (8.16).

The eigenvalue of the number operator \hat{N} will be denoted by N , and it is clear from (8.16) that it is given by

$$N = 2n + \ell. \quad (38.5)$$

It will prove convenient to use not only the angular ket notation $|nlm\rangle$ for the states (8.16) but also by the round ket notation in which the total quantum number N appears, *i.e.*,

$$|N\ell m\rangle = |n\ell m\rangle, \quad (38.6)$$

where the relation (38.5) holds.

Furthermore instead of the cartesian creation and annihilation operators (8.8), which we shall now denote here as $\bar{\eta}_i, \bar{\xi}_i$, we will like to use them in terms of spherical components

$$\eta_p, \xi^q, \quad p, q = 1, 0, -1, \quad (38.7)$$

where

$$\eta_1 = -\frac{1}{\sqrt{2}}(\bar{\eta}_1 + i\bar{\eta}_2), \quad \eta_0 = \bar{\eta}_3, \quad \eta_{-1} = \frac{1}{\sqrt{2}}(\bar{\eta}_1 - i\bar{\eta}_2), \quad (38.8)$$

and

$$\xi^p = (-1)^p \xi_{-p} = \eta_p^\dagger, \quad \text{with} \quad \bar{\eta}_i^\dagger = \bar{\xi}_i, \quad (38.9)$$

where we use covariant and contravariant indices as now the metric is not euclidean, *i.e.*, given by δ_{ij} , but instead it is $(-1)^p \delta_{p,-q}$.

The generators of the U(3) group can now be denoted by

$$C_p^q = \eta_p \xi^q, \quad (38.10)$$

and those of the O(3) subgroup are seen from (8.15), again in spherical components to have the form

$$L_1 = -(C_1^0 + C_0^{-1}), \quad (38.11a)$$

$$L_0 = (C_1^1 - C_{-1}^{-1}), \quad (38.11b)$$

$$L_{-1} = (C_{-1}^0 + C_0^1), \quad (38.11c)$$

or

$$L_r = \sqrt{6} \sum_{p,q} (-1)^q \begin{pmatrix} 1 & 1 & 1 \\ p & r & -q \end{pmatrix} C_q^p. \quad (38.11d)$$

Finally to complete what we could call the Racah tensor form of the generators of U(3) we could define

$$Q_m = \sum_{p,q=-1}^1 (-1)^{q-1} \sqrt{3} \begin{pmatrix} 1 & 2 & 1 \\ p & m & -q \end{pmatrix} C_q^p, \quad (38.12)$$

which has five components as $m = 2, 1, 0, -1, -2$.

If we have now n particles instead of one, we have to add to the creation and annihilation operators a lower index s , *i.e.*,

$$\eta_{ps}, \xi_s^q, \quad p, q = 1, 0, -1, \quad s = 1, 2, \dots n, \quad (38.13)$$

and now the generators of U(3) continue to be denoted by (38.10) but with a sum with respect to the index s over its values $s = 1, 2, \dots n$. The total angular momentum $L_q, q = 1, 0, -1$, and the second rank Racah tensor $Q_m, m = 2, 1, 0, -1, -2$, continue to be given by the relations (38.11) and (38.12).

Let us now turn from the one to the two-body problem in the chain (38.1) which could be completed by appropriate orthogonal subalgebras, *i.e.*,

$$\begin{array}{ccccc} & N_1 & & N_2 & \\ u(6) \supset & u_1(3) & \oplus & u_2(3) & \\ & \cup & & \cup & \\ & \ell_1 & o_1(3) & o_2(3) & \ell_2 \\ & & \searrow & \downarrow & \\ & & o_{12}(3) & & \Lambda \end{array} \quad (38.14)$$

The states corresponding to this chain are exactly those given in Eq. (10.10) of this book, only that it is better to use the round bracket notation defined in (38.6) and write them as the ket

$$|N_1 \ell_1, N_2 \ell_2, \Lambda M\rangle, \quad (38.15a)$$

with $N_s = 2n_s + \ell_s, s = 1, 2$. We have put on top of the Lie algebras $u_1(3), u_2(3)$ in (38.14) the numbers N_1, N_2 that characterize their irreducible representation and correspondingly on the left and right of $o_1(3), o_2(3)$ and below $o_{12}(3)$ the values ℓ_1, ℓ_2, Λ .

The states (38.15a) were discussed extensively in Chapter II so we do not need to analyze them further. It is good though to use the full bracket notation of Dirac and write them as

$$(\eta_1, \eta_2 | N_1 \ell_1, N_2 \ell_2, \Lambda M) \quad (38.15b)$$

to stress the fact that we are dealing with *two* particles whose creation operators are η_1 and η_2 .

As we show in section 17, we can deal with a *three* particle problem in relative motion by considering the state (17.5), (17.6) which means that we replace in (38.15b), η_1, η_2 by the Jacobi ones for three particles:

$$\dot{\eta}_1 = (1/\sqrt{2})(\eta_1 - \eta_2), \quad \dot{\eta}_2 = (1/\sqrt{6})(\eta_1 + \eta_2 - 2\eta_3), \quad (38.16)$$

so that we have the round brackets

$$(\dot{\eta}_1 \dot{\eta}_2 | N_1 \ell_1, N_2 \ell_2, \Lambda M). \quad (38.17)$$

It is then relevant to characterize them also by irreducible representations of the permutation group of three particles and this is done in detail in section 17.

It is clear that the chain (38.14) of Lie algebras can be generalized straightforwardly to an arbitrary number of particles by just coupling the angular momenta through intermediate steps as done, for example, in Eq. (21.2). Thus it is not worthwhile to discuss in the chain (38.1) examples in which $n > 2$.

b) States for the chain (38.3)

It is clear that the chains (38.1) and (38.3) are identical if $n = 1$, so this case was already discussed in the previous example. The first interesting case is then $n = 2$ and as we are still concerned with states of total angular momentum, we can consider the chain of groups

$$\begin{array}{c} \text{U(6)} \supset \text{U(3)} \otimes \text{U(2)} \\ \cup \quad \cup \\ \text{O(3)} \quad \text{SU(2)} \\ \cup \quad \cup \\ \text{O(2)} \quad \text{O(2)}. \end{array} \quad (38.18)$$

The subgroups of U(3) are the same than those that we used in the previous subsection and the generators of U(3), O(3), O(2) are respectively C_p^q , $p, q = 1, 0, -1$, of (38.10), L_q , $q = 1, 0, -1$, of (38.11) and L_0 also of (38.11b).

The generators of U(2) are the C_{st} , $s, t = 1, 2$ of (37.14b). This group of two-dimensional unitary matrices has as a subgroup the one when all those matrices have determinant 1, which is known as SU(2) and whose generators can be written as

$$\hat{F}_+ \equiv C_{12}, \quad (38.19a)$$

$$\hat{F}_0 = (1/2)(C_{11} - C_{22}), \quad (38.19b)$$

$$\hat{F}_- = C_{21}, \quad (38.19c)$$

which satisfy the commutation relations

$$[\hat{F}_0, \hat{F}_{\pm}] = \pm \hat{F}_{\pm}, \quad [\hat{F}_+, \hat{F}_-] = 2\hat{F}_0, \quad (38.20)$$

Besides there is a generator that commutes with all of those in (38.20), i.e., a Casimir operator which is related to the number of quanta, i.e.,

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$$\hat{N} \equiv C_{11} + C_{22} = C_1^1 + C_0^0 + C_{-1}^{-1}, = \sum_{p,q} (-1)^{q+1} \sqrt{3} \begin{pmatrix} 1 & 0 & 1 \\ p & 0 & -q \end{pmatrix} C_q^p, \quad (38.21)$$

where the right hand side in the expression comes from the relation $\Gamma_1 = \Delta_1$ in (37.19a).

We can restrict ourselves then to the U(2) group where

$$\Delta_1 = \hat{N} = \Gamma_1 \quad (38.22a)$$

$$\Delta_2 = \sum_{s,t=1}^2 C_{st} C_{ts} = (1/2)\hat{N}^2 + 2\hat{F}^2, \quad (38.22b)$$

where

$$\hat{F}^2 = \hat{F}_- \hat{F}_+ + \hat{F}_0(\hat{F}_0 + 1), \quad (38.23)$$

while all Δ_n with $n > 2$ are functions of \hat{N}^2, \hat{F}^2 so they provide no further information.

The irreducible representations (irreps) of $\text{U}(3) \otimes \text{U}(2)$ are then characterized by the eigenvalues of the operators \hat{N} and \hat{F}^2 . For the former this is N the number quanta, for the latter, as the commutation rules are the same as those of the angular momentum, the eigenvalue can be expressed in the form

$$\mathcal{F}(\mathcal{F} + 1), \quad (38.24)$$

where \mathcal{F} is a nonnegative integer or semi-integer.

The irreps of U(3) for the two particle problem can then be characterized by

$$N, \mathcal{F}. \quad (38.25)$$

Note that in (38.18) SU(2) has an orthogonal subgroup O(2) whose generator is \hat{F}_0 of (38.19b) and where we shall designate its eigenvalue by ν . As N_1, N_2 , the numbers of quanta for particles 1 and 2 are respectively the eigenvalues of C_{11}, C_{22} we get

$$N = N_1 + N_2, \quad \nu = (1/2)(N_1 - N_2). \quad (38.26)$$

For a fixed N , the maximum value of ν is $(N/2)$ corresponding to $N_1 = N, N_2 = 0$. As $\nu = \mathcal{F}, \mathcal{F} - 1, \dots, -\mathcal{F}$, we see that the maximum value of \mathcal{F} is also $(N/2)$ and from there it can only diminish by integral steps.

As the irrep of $O(3)$, $O(2)$ are characterized by Λ, M respectively we could now characterize a state related to the chain (38.18) by $N, \mathcal{F}, \nu, \Lambda, M$. Since the pioneer work of Elliott [13,14] it has been customary to replace N, \mathcal{F} by the numbers λ, μ defined by

$$\lambda = 2\mathcal{F}, \quad \mu = (N/2) - \mathcal{F}, \quad (38.27)$$

and we shall then characterize a ket that is part of a basis for an irrep of the chain (38.18) by

$$\left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & M \end{array}; \nu \right\rangle = P_{(\lambda\mu)\alpha\Lambda M\nu}(\eta_1, \eta_2)|0\rangle, \quad (38.28)$$

where P is a homogeneous polynomial of degree $\lambda + 2\mu$ in the components of the creation operators η_1 , and η_2 and $|0\rangle$ the ground state (10.12). Note the appearance of an α , as yet undefined, that is needed to distinguish repeated irreps of $O(3)$ of given Λ in a definite irrep $(\lambda\mu)$ of $U(3)$.

Our problem now is to find explicitly the state (38.28) which means the determination of the corresponding polynomial. For this purpose we note that we could restrict ourselves to states with $M = \Lambda, \nu = \mathcal{F} = (\lambda/2)$ as the more general one in (38.28) could be obtained from the one mentioned if we apply powers of the lowering operators C_{21} and L_{-1} .

Thus we concentrate on a state that we could denote as [15,16]

$$\left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = P_{(\lambda\mu)\alpha\Lambda}(\eta_1, \eta_2)|0\rangle, \quad (38.29)$$

where we suppressed the $\nu = \mathcal{F} = (\lambda/2)$ and $M = \Lambda$ as they are redundant, and which satisfies the following equations [16]

$$C_{11} \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = (\lambda + \mu) \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle, \quad (38.30a)$$

$$C_{22} \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = \mu \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle, \quad (38.30b)$$

$$C_{12} \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = 0 \quad (38.30c)$$

$$L_1 \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = 0, \quad (38.30d)$$

$$L_0 \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle = \Lambda \left| \begin{array}{ccc} \lambda & \mu & \\ \alpha & \Lambda & \end{array} \right\rangle. \quad (38.30e)$$

We note that all of these operators contain linearly ξ_s^q , $q = 1, 0, -1$, $s = 1, 2$, and as

$$[\xi_s^q, \eta_{rt}] = \delta^{st} \delta_r^q, \quad (38.31)$$

we could consider, when acting on the polynomial $P_{(\lambda\mu)\alpha\Lambda}(\eta_1, \eta_2)$ in (38.29), that the ξ_s^q behaves as the first order differential operator

$$\xi_s^q \rightarrow \frac{\partial}{\partial \eta_{qs}}. \quad (38.32)$$

Thus if we find a set of solutions of Eq. (38.30), a product of powers of these solutions is also a solution.

In view of the last phrase our first objective will be to find what are called elementary permissible diagrams (epd) [17], i.e., solution of Eq. (38.30), that cannot be reduced to products of powers of simpler solutions. By trial and error we immediately find five of these epd's:

$$\eta_+ \equiv \eta_{11}, \quad \left(\begin{array}{ccc} \lambda & \mu & \Lambda \\ 1 & 0 & 1 \end{array} \right), \quad (38.33a)$$

$$v_+ \equiv (\eta_1 \times \eta_2)_1, \quad (0 \ 1 \ 1), \quad (38.33b)$$

$$w_+ \equiv [(\eta_1 \times \eta_2) \times \eta_1]_1, \quad (1 \ 1 \ 1), \quad (38.33c)$$

$$s = (\eta_1 \cdot \eta_1), \quad (2 \ 0 \ 0), \quad (38.33d)$$

$$t = [(\eta_1 \times \eta_2) \cdot (\eta_1 \times \eta_2)], \quad (0 \ 2 \ 0), \quad (38.33e)$$

with the \times indicating vector product and the corresponding values of $(\lambda\mu\Lambda)$ indicated on the right hand side.

Obviously the application L_1 to all of these expressions gives 0 as they are of highest projection in their angular momentum. The same happens when we apply C_{12} which implies changing the index 2 to 1. As for C_{11}, C_{22} we have that

$$C_{11}\eta_+ = \eta_+, \quad C_{11}v_+ = v_+, \quad C_{11}w_+ = 2w_+, \\ C_{11}s = 2s, \quad C_{11}t = 2t, \quad (38.34a)$$

$$C_{22}\eta_+ = 0, \quad C_{22}v_+ = v_+, \quad C_{22}w_+ = w_+, \\ C_{22}s = 0, \quad C_{22}t = 2t. \quad (38.34b)$$

Only the w_+ has to remain of power 1 as

$$w_+^2 = -(\eta_+^2 t + v_+^2 s), \quad (38.35)$$

and so is expressible in terms of the others. Thus we easily check that the states (38.29) that satisfy (38.30) can be written in terms of products of

powers of the operators (38.33) as

$$\begin{pmatrix} \lambda & \mu \\ \alpha & \Lambda \end{pmatrix} = \eta_+^\alpha v_+^{\Lambda-\alpha} s^{\frac{1}{2}(\lambda-\alpha)} t^{\frac{1}{2}(\mu-\Lambda+\alpha)} |0\rangle, \\ \text{if } \lambda + \mu - \Lambda \text{ even,} \quad (38.36a)$$

$$\begin{pmatrix} \lambda & \mu \\ \alpha & \Lambda \end{pmatrix} = \eta_+^{\alpha-1} v_+^{\Lambda-\alpha} w_+ s^{\frac{1}{2}(\lambda-\alpha)} t^{\frac{1}{2}(\mu-\Lambda+\alpha-1)} |0\rangle, \\ \text{if } \lambda + \mu - \Lambda \text{ odd.} \quad (38.36b)$$

The range of α, Λ in (38.36) are determined by the fact that the exponents are all nonnegative integers. Thus α takes integer values with the parity of λ in the range

$$\max(0, \Lambda - \mu) \leq \alpha \leq \min(\Lambda, \lambda), \quad (38.37)$$

except that there is no $\alpha = 0$ for $(\mu - \Lambda)$ odd.

It is easily verified that the states (38.36) are linearly independent [17] and that together with states of M lower than $M = \Lambda$, obtained by cranking down with powers of L_{-1} , they give the correct number of states [17] characterized by the irrep $(\lambda\mu)$ of $U(3)$, i.e.,

$$(1/2)(\lambda+1)(\mu+1)(\lambda+\mu+2). \quad (38.38)$$

In Table VII.1 we give the possible values of the angular momenta for given $(\lambda\mu)$ as well as the values of N, \mathcal{F} for N up to 12 quanta and where an exponent appears in the value of Λ , it indicates the number of times it is repeated.

As both (38.28) and (38.15) form a complete set we can develop one in terms of the other, i.e., find the brackets

$$\left(N_1 \ell_1, N_2 \ell_2, \Lambda M \middle| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda & M \\ \nu \end{matrix} \right), \quad (38.39)$$

where

$$N_1 + N_2 = \lambda + 2\mu, \quad (38.40a)$$

$$(1/2)(N_1 - N_2) = \nu. \quad (38.40b)$$

This bracket is independent [18] of M as the subgroup $O(2)$ appears in both chains of groups, so we could put $M = \Lambda$ or suppress it altogether in the bracket. Furthermore if we take for ν its highest value, i.e.,

$$\nu = \mathcal{F} = (\lambda/2), \quad (38.41)$$

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Table VII.1. Values of the angular momentum Λ compatible with a given irrep (λ,μ) of $SU(3)$, where $N = \lambda + 2\mu$, $\mathcal{F} = (\lambda/2)$.

(λ, μ)	N	\mathcal{F}	Λ
(0,0)	0	0	0
(1,0)	1	1/2	1
(2,0)	2	1	0,2
(0,1)	0	1	
(3,0)	3	3/2	1,3
(1,1)		1/2	1,2
(4,0)	4	2	0,2,4
(2,1)		1	1,2,3
(0,2)	0	0,2	
(5,0)	5	5/2	1,3,5
(3,1)		3/2	1,2,3,4
(1,2)		1/2	1,2,3
(6,0)	6	3	0,2,4,6
(4,1)		2	1,2,3,4,5
(2,2)		1	0,(2) ² ,3,4
(0,3)	0	0,1,3	
(7,0)	7	7/2	1,3,5,7
(5,1)		5/2	1,2,3,4,5,6
(3,2)		3/2	1,2,(3) ² ,4,5
(1,3)		1/2	1,2,3,4
(8,0)	8	4	0,2,4,6,8
(6,1)		3	1,2,3,4,5,6,7
(4,2)		2	0,(2) ² ,3,(4) ² ,5,6
(2,3)		1	1,2,(3) ² ,4,5
(0,4)	0	0,2,4	
(9,0)	9	9/2	1,3,5,7,9
(7,1)		7/2	1,2,3,4,5,6,7,8
(5,2)		5/2	1,2,(3) ² ,4,(5) ² ,6,7
(3,3)		3/2	1,2,(3) ² ,(4) ² ,5,6
(1,4)		1/2	1,2,3,4,5
(10,0)	10	5	0,2,4,6,8,10
(8,1)		4	1,2,3,4,5,6,7,8,9
(6,2)		3	0,(2) ² ,3,(4) ² ,5,(6) ² ,7,8
(4,3)		2	1,2,(3) ² ,(4) ² ,(5) ² ,6,7
(2,4)		1	0,(2) ² ,3,(4) ² ,5,6
(0,5)	0	0,1,3,5	
(11,0)	11	11/2	1,3,5,7,9,11
(9,1)		9/2	1,2,3,4,5,6,7,8,9,10
(7,2)		7/2	1,2,(3) ² ,4,(5) ² ,6,(7) ² ,8,9
(5,3)		5/2	1,2,(3) ² ,(4) ² ,(5) ² ,(6) ² ,7,8
(3,4)		3/2	1,2,(3) ² ,(4) ² ,(5) ² ,6,7
(1,5)		1/2	1,2,3,4,5,6
(12,0)	12	6	0,2,4,6,8,10,12
(10,1)		5	1,2,3,4,5,6,7,8,9,10,11
(8,2)		4	0,(2) ² ,3,(4) ² ,5,(6) ² ,7,(8) ² ,9,10
(6,3)		3	1,2,(3) ² ,(4) ² ,(5) ² ,(6) ² ,(7) ² ,8,9
(4,4)		2	0,(2) ² ,3,(4) ² ,(5) ² ,(6) ² ,7,8
(2,5)		1	1,2,(3) ² ,4,(5) ² ,6,7
(0,6)	0	0,2,4,6	

then we have

$$N_1 = \lambda + \mu, \quad (38.42a)$$

$$N_2 = \mu, \quad (38.42b)$$

and as the index ν is redundant we could write (38.39) as

$$\left(\lambda + \mu \ l_1, \ \mu \ l_2, \ \Lambda \middle| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix} \right), \quad (38.43)$$

where the ket is given by (38.36) and the bra by (38.15) with $M = \Lambda$ and N_1, N_2 replaced by their values in (38.42). This bracket is explicitly calculated in reference [17] and it is known as a reduced Wigner coefficient for the $U(3) \supset O(3)$ chain.

So far we have spoken of ket (38.28) associated with the chain of groups (38.3) in terms of the components of the creation operator vectors of two particles η_1, η_2 , i.e., in full bracket notation of

$$\left\langle \eta_1, \eta_2 \middle| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix} \ M; \nu \right\rangle, \quad (38.44)$$

which corresponds to (38.15) for the chain (38.1).

Using the Jacobi vectors (38.16) we could extend our analysis to a system of three particles in relative motion by just writing

$$\left\langle \dot{\eta}_1, \dot{\eta}_2 \middle| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix} \ M; \nu \right\rangle. \quad (38.45)$$

It is then relevant to characterize these states also by the permutation group of these three particles, which can be done in a similar to the way we proceeded in Section 17.

As a final point we wish to stress that the states (38.36), that are a basis for the irreducible representation of the chain of groups (38.18), is complete but not orthonormal, due to the purely algebraic significance of the index α of (38.37). We can though orthonormalize these states by applying to them the hermitian operator

$$\Omega = \sum_{\substack{p,q=-1 \\ m=p+q}}^1 (-1)^m \sqrt{5} \begin{pmatrix} 1 & 1 & 2 \\ p & q & -m \end{pmatrix} L_p L_q Q^m, \quad (38.46)$$

which from (38.11) and (38.12) is in the enveloping algebra of $U(3)$ and besides, because of the $3j$ coefficient in (38.46), is a scalar of $O(3)$. Thus when applied to the states (38.36) it can only change the index α , and thus

it provides a numerical and finite matrix [16] acting on the states $\left| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix} \right\rangle$, whose determinant gives the eigenvalues of Ω , that are all different [16]. For each one of them we get an eigenvector with which we can form the linear combination of states $\left| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix} \right\rangle$ that are orthonormal.

Other procedures for orthonormalizing the states have been presented in the literature based on a method suggested by Elliott [13].

39 Application of the $U(3)$ States in the 2s-1d Nuclear Shell

In section 13 we found many uses in nuclear shell theory for the two particle states characterized by the chain of groups (38.14), when combined with the spin-isospin part of the state.

We have not yet discussed any application of the two particle states characterized by the chain (38.18), but we shall proceed to do this in the present section. We start by noting that the central interaction between two particles can be developed in the following fashion:

$$V(|\mathbf{r}_1 - \mathbf{r}_2|) = \sum_{k=0}^{\infty} V_k(r_1, r_2) P_k(\cos \Theta_{12}), \quad (39.1)$$

where P_k is a Legendre polynomial and Θ_{12} the angle between the vector \mathbf{r}_1 and \mathbf{r}_2 .

If the range of this potential is large compared with the dimensions of the region where our states are concentrated or, equivalently, when we use units $\hbar = m = \omega = 1$, if this range is much larger than 1, the $V_k(r_1, r_2)$ which depends on the magnitudes of the vectors $\mathbf{r}_1, \mathbf{r}_2$ can be expanded in powers of r_1, r_2 , and $P_k(\cos \Theta_{12})$ can also be developed in terms of the spherical harmonics of particles 1 and 2, so we get a quickly convergent series of terms whose general form is

$$\sum_{\tau=-k}^k r_1^{k+m} Y_{k\tau}(\theta_1, \phi_1) r_2^{k+n} Y_{k\tau}^*(\theta_2, \phi_2). \quad (39.2)$$

If we limit ourselves to powers of r_1 and r_2 not larger than 2, we see that the possibilities when $k = 0$, either just add a constant to the energy or modify the frequency of our oscillator or make it anharmonic, all of which does not change the essential character of our spectra. The terms with $k = 1$ will vanish for parity reasons if we consider its matrix elements for states

of the type (38.15) restricted to a single shell, *i.e.*, when $N_1 = N_2$ in both bra and ket. Thus the first relevant type of interaction will be of the form

$$\sum_{m=-2}^2 r_1^2 Y_{2m}(\theta_1, \phi_1) r_2^2 Y_{2m}^*(\theta_2, \phi_2), \quad (39.3)$$

i.e., a quadrupole-quadrupole one. We can write

$$r_s^2 Y_{2m}(\theta_s, \phi_s) = -\frac{5}{\sqrt{8\pi}} \sum_{p,q} (-1)^{q-1} \sqrt{3} \begin{pmatrix} 1 & 2 & 1 \\ p & m & -q \end{pmatrix} x_s^p x_{qs}, \quad (39.4a)$$

where x_{qs} , $q = 1, 0, -1$ are the spherical components of \mathbf{r}_s , $s = 1, 2$.

As

$$x_{qs} = \frac{1}{\sqrt{2}} (\eta_{qs} + \xi_{qs}), \quad (39.4b)$$

if we substitute it in (39.4a) and keep only the terms that do not change the number of quanta for the states of each particle, *i.e.*, that are of the form $\eta_s^p \xi_{qs}$ or $\xi_s^p \eta_{qs}$, we see that we can replace the term in (39.4) by

$$-\frac{5}{2\sqrt{2\pi}} (Q_m)_s, \quad (39.5)$$

where Q_m is given by (38.12) but restricted to particle s .

The quadrupole-quadrupole interaction (39.3) for states in a single shell, becomes then proportional to the product of $(Q_m)_1$ and $(Q_m)_2$ and it can be generalized to the expression

$$Q^2 = \sum_{m=-2}^2 (-1)^m Q_m Q_{-m}, \quad (39.6)$$

where now Q_m is defined by (38.12) but with C_p^q summed over the particle index s .

If the potential between the particles is attractive Q^2 will be multiplied by a negative constant, and we could think of a two particle Hamiltonian in an oscillator potential with a long range interaction [14] given by

$$H = H_0 - (Q^2/\mathcal{I}), \quad (39.7)$$

where H_0 is the kinetic energy plus oscillator potential terms for the two particles.

It turns out then that the eigenvalues of the potential (39.7) can be obtained exactly as, from their definitions, it is easily shown that $\Gamma_2 = (5/3)Q^2 + (1/3)N^2 + (1/2)L^2$, so from (37.19b) we get

$$Q^2 = \frac{3}{5}\Delta_2 - \frac{1}{5}\Delta_1^2 + \frac{3}{5}\Delta_1 - \frac{3}{10}L^2, \quad (39.8)$$

and so from (38.22) we see that the eigenvalue E of (39.7) becomes

$$E = N - \mathcal{I}^{-1} \left\{ \frac{3}{10}N^2 + \frac{6}{5}\mathcal{F}(\mathcal{F}+1) - \frac{1}{5}N^2 + \frac{3}{5}N - \frac{3}{10}\Lambda(\Lambda+1) \right\}, \quad (39.9)$$

while the eigenstates are precisely those characterized by the basis of the irrep of the U(3) group given in (38.28) and that can be obtained from the explicit expressions (38.36) after applying to them powers of the lowering operators L_{-1} and C_{21} .

The main importance of the states (38.36) is not though in the fact that for them eigenvalues of the Hamiltonian (39.7) can be expressed in an explicitly analytic fashion, but that states corresponding to given irrep of U(3) contribute a large part of the lowest states for shell model calculation such as those discussed in section 14 of this book. To derive this result we should also include in our U(3) states (38.28) the spin and isospin so that we finally can write kets of the form

$$\begin{aligned} \left| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix}; SJM; \nu TM_T \right\rangle &= \left\{ \sum_{M_\Lambda M_S} (-1)^{\Lambda-S+M} \sqrt{2J+1} \times \right. \\ &\times \left. \left(\begin{matrix} \Lambda & S & J \\ M_\Lambda & M_S & -M \end{matrix} \right) \left| \begin{matrix} \lambda & \mu \\ \alpha & \Lambda \end{matrix}; M_\Lambda; \nu \right\rangle \left| \begin{matrix} \frac{1}{2} & \frac{1}{2} \\ S & M_S \end{matrix} \right\rangle \right\} \left| \begin{matrix} \frac{1}{2} & \frac{1}{2} \\ T & M_T \end{matrix} \right\rangle, \end{aligned} \quad (39.10)$$

where on the right hand side the first ket is given by (38.28), the second corresponds to two spins 1/2 coupled to a total one $S = 0, 1$ and the third to two isospins 1/2 coupled to $T = 0, 1$.

Considering then the $j-j$ coupling shell states of section 14 we can evaluate their scalar product with those in (39.10), as both involve polynomials in the creation operators acting on the ground state. The square of the absolute values of these scalar products give the percentage of the state (39.10) present in those discussed in section 14 and this value was obtained by Elliott [13,14] and is given below for two nucleons outside the closed shell of ^{16}O :

Nucleus	T	J	$(\lambda\mu)\Lambda$	%U(3)
^{18}F	0	1	(40)0	92
	0	3	(40)2	96
	0	5	(40)4	100 trivial
^{18}O	1	0	(40)0	72
	1	2	(40)2	72

(39.11)

From this table one clearly sees the preponderance of the state (40), the symmetric representation of U(3), in those derived in section 14, which, incidentally, were also based on a work of Elliott and Flowers (see section 14), but used the concept of transformation brackets of section 10 to simplify the calculations.

So far we have been discussing only two particle problems in the U(3) representation, but actually the analysis applied to derive them can be generalized to n particles. We proceed to outline it here, as Elliott [13,14], and a large group of physicists in the sixties, applied them extensively for nuclei in the 2s-1d shell.

We consider the chain of groups

$$\begin{aligned} \text{U}(3n) &\supset \text{U}(3) \otimes \text{U}(n) \\ &\cup \\ &\text{O}(3) \\ &\cup \\ &\text{O}(2), \end{aligned} \quad (39.12)$$

where for the moment we do not specify the chain of subgroups of U(n). We wish though to note that the generators C_{st} , $s, t = 1, 2, \dots, n$, defined in (37.14b), can be grouped in three sets:

$$C_{st}, s < t; \quad C_{st}, s = t; \quad C_{st}, s > t, \quad (39.13)$$

which in the literature [19] are known respectively as those that raise, give and lower the weight. This is analogous to L_+ , L_0 and L_- for O(3), where L_0 give the weight, i.e., the eigenvalue, m of the state, while L_+ , when applied to the state, raises the weight to $m+1$ while L_- lowers it to $m-1$.

Now, when discussing the chain (39.12) we could consider first the states of highest weight in U(n), i.e., that vanish if C_{st} with $s < t$ is applied to them. For those states we can specify the weight by applying the operators $C_{ss} = 1, 2, \dots, n$ to them, and get eigenvalues we could denote by h_s , $s = 1, 2, \dots, n$, and the set $[h_1 h_2 \dots h_n]$ characterizes the irrep of U(n) and thus also of U(3) as they are complementary. For the group O(3) we also consider it of highest weight, i.e., when L_+ applied to it gives zero. Thus we have the ket

39. APPLICATION OF THE U(3) STATES

$$\left| \begin{matrix} [h_1 h_2 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle = P_{[h_1 \dots h_n]\alpha\Lambda}(\eta_1, \eta_2 \dots \eta_n) |0\rangle, \quad (39.14)$$

which satisfies the equations

$$C_{ss} \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle = h_s \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle, \quad (39.15a)$$

$$C_{st} \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle = 0 \quad \text{if } s < t; \quad (39.15b)$$

$$L_+ \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle = 0, \quad (39.16a)$$

$$L_0 \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle = \Lambda \left| \begin{matrix} [h_1 \dots h_n] \\ \alpha\Lambda \end{matrix} \right\rangle. \quad (39.16b)$$

We first consider (39.15b) when $t \geq 4$. In that case, considering the differential character of the operator ξ_i^s indicated in (38.32), we see that the polynomial P satisfies the following equations:

$$\eta^1 \cdot \frac{\partial P}{\partial \eta^t} = 0, \quad \eta^2 \cdot \frac{\partial P}{\partial \eta^t} = 0, \quad \eta^3 \cdot \frac{\partial P}{\partial \eta^t} = 0, \quad (39.17)$$

i.e., three homogeneous equations for the partial derivatives $(\partial P / \partial \eta_q^t)$, $q = 1, 0, -1$, $t \geq 4$, with determinant

$$D = (\eta_1 \times \eta_2) \cdot \eta_3, \quad (39.18)$$

which is clearly different from 0. Thus,

$$(\partial P / \partial \eta_q^t) = 0 \quad \text{if } q = 1, 0, -1, t \geq 4, \quad (39.19)$$

and P depends only on η_1, η_2, η_3 , so $h_t = 0$ if $t \geq 4$.

For $t = 3$ we have the three equations

$$\eta_1 \cdot \frac{\partial P}{\partial \eta_3} = 0, \quad \eta_2 \cdot \frac{\partial P}{\partial \eta_3} = 0, \quad \eta_3 \cdot \frac{\partial P}{\partial \eta_3} = h_3 P, \quad (39.20)$$

and to see the restriction it imposes on P we introduce the rational function

$$R(\eta_1, \eta_2, \eta_3) = D^{-h_3} P(\eta_1, \eta_2, \eta_3). \quad (39.21)$$

Expressing P in terms of R and substituting it in (39.20) we get

$$\eta_s \cdot \frac{\partial R}{\partial \eta_3} = 0, \quad s = 1, 2, 3, \quad (39.22)$$

which implies that R is independent of η_3 , so finally we may write

$$P(\eta_1, \eta_2, \eta_3) = D^{h_3} \frac{u(\eta_1, \eta_2)}{v(\eta_1, \eta_2)}, \quad (39.23)$$

where we replaced the rational function R of just η_1, η_2 by a ratio of two polynomials in these same variables that have no common factor. We use now the well known algebraic fact that the determinant is not divisible by a polynomial (except a constant) to conclude that v is a constant since it is relatively prime to both factors of the numerator in Eq. (39.23). Absorbing the constant in u we can write

$$P(\eta_1, \eta_2, \eta_3) = [(\eta_1 \times \eta_2) \cdot \eta_3]^{h_3} u(\eta_1, \eta_2), \quad (39.24)$$

and $u(\eta_1, \eta_2)$ satisfies exactly the same equations as those of (38.30). Thus the polynomial of highest weight in (39.14) is given by the one appearing in (38.36) multiplied by D^{h_3} .

Introducing now the notation $\lambda = h_1 - h_2$, $\mu = h_2 - h_3$, $\rho = h_3$, we can denote the state (39.14) as

$$\begin{vmatrix} \lambda & \mu & \rho \\ \alpha & \Lambda \end{vmatrix} = P_{\lambda\mu\alpha\Lambda}(\eta_1, \eta_2)[(\eta_1 \times \eta_2) \cdot \eta_3]^{\rho}|0\rangle, \quad (39.25)$$

where $P_{(\lambda\mu)\alpha\Lambda}$ is the one appearing in (38.29) and given by (38.36).

Once we have what we could call the highest weight state in $U(n)$ and $O(3)$ in the chain (39.12), we can get all others by applying products of powers of the lowering operators C_{st} , $s > t$, as well as powers of L_{-1} .

This procedure, while feasible, is tedious and not physically significant. In a paper of Kramer and Moshinsky [20] entitled "Group Theory of Harmonic Oscillators and Nuclear Structure" it is systematized so as to have an appropriate set of subgroups of $U(n)$ ending in the symmetric group of S_n of n particles. Not only the states are explicitly constructed, but the fractional parentage coefficients are obtained, to be able to calculate matrix elements of Hamiltonians and of other relevant operators. Applications can then be made in the 2s-1d nuclear shell model for systems of more than two particles outside the closed shell of ^{16}O .

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Chapter VIII

Four-Dimensional Harmonic Oscillator and Coulomb Problem

40 Four-Dimensional Harmonic Oscillator and Its Eigenvalues and Eigenfunctions

In this chapter we are interested in a four-dimensional harmonic oscillator (FDHO). Also the wave functions of one-, two- and three-dimensional harmonic oscillators are used. In this connection we begin with a description of general properties of the harmonic oscillator in a space of any dimension d . Then we concretize these results for special case $d = 4$.

The Hamiltonian of the d -dimensional harmonic oscillator is of the form

$$H^{\text{osc}} = \sum_{k=1}^d \left(\frac{p_k'^2}{2m} + \frac{m\omega^2 x_k'^2}{2} \right), \quad (40.1)$$

where

$$p'_k = -i\hbar \frac{\partial}{\partial x'_k}, \quad k = 1, 2, \dots, d, \quad (40.2)$$

are components of the d -dimensional momentum. If we introduce dimensionless variables

$$x_k = \frac{x'_k}{r_0}, \quad r_0 = \left(\frac{\hbar}{m\omega} \right)^{1/2}, \quad (40.3)$$

the Schrödinger equation for this oscillator can be written in the form

$$\left(-\frac{1}{2}\Delta_d + \frac{1}{2}\rho^2 \right) \Psi(x_k) = E\Psi(x_k). \quad (40.4)$$

Here,

$$\rho^2 = \sum_{k=1}^d x_k^2 \quad (40.5)$$

is a square of the d -dimension radius vector and

$$\Delta_d = \sum_k \frac{\partial^2}{\partial x_k^2} \quad (40.6)$$

is a d -dimensional Laplace operator.

Equation (40.4) is separable in d -dimensional hyperspherical coordinates $\rho, \theta_1, \theta_2, \dots, \theta_{d-1}$. The choice of the angle variables in two- and three-dimensional cases is standard: polar and spherical angles respectively. At $d = 4$ we use the four-dimensional spherical coordinates which are connected with Cartesian coordinates x_k as follows:

$$\begin{aligned} x_1 &= \rho_1 \cos \alpha, \quad 0 \leq \alpha < 2\pi, \\ x_2 &= \rho_1 \sin \alpha, \\ x_3 &= \rho_2 \cos \gamma, \quad 0 \leq \gamma < 2\pi, \\ x_4 &= \rho_2 \sin \gamma, \\ \rho_1 &= \rho \cos \beta, \quad 0 \leq \beta \leq \frac{\pi}{2}, \\ \rho_2 &= \rho \sin \beta. \end{aligned} \quad (40.7)$$

In hyperspherical coordinates Eq. (40.4) takes the form

$$\begin{aligned} \frac{1}{2} \left(-\frac{1}{\rho^{d-1}} \frac{\partial}{\partial \rho} \left(\rho^{d-1} \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \Delta_\Omega + \rho^2 \right) \Psi(\rho, \theta_i) \\ = E\Psi(\rho, \theta_i). \end{aligned} \quad (40.8)$$

The angular part of the four-dimensional Laplace operator in variables (40.7) is given by the expression [1]

$$\begin{aligned} \Delta_\Omega &= \frac{1}{\sin \beta \cos \beta} \frac{\partial}{\partial \beta} \left(\sin \beta \cos \beta \frac{\partial}{\partial \beta} \right) \\ &+ \frac{1}{\sin^2 \beta} \frac{\partial^2}{\partial \alpha^2} + \frac{1}{\cos^2 \beta} \frac{\partial^2}{\partial \gamma^2}. \end{aligned} \quad (40.9)$$

The wave function in Eq. (40.8) can be represented as a product of the radial and angular functions:

$$\Psi(\rho, \theta_i) = R(\rho)Y(\theta_i). \quad (40.10)$$

The d -dimensional spherical harmonic $Y(\theta_i)$ is an eigenfunction of the angular part of the Laplace operator

$$\Delta_\Omega Y(\theta_i) = \lambda Y(\theta_i), \quad \lambda = -K(K+d-2), \quad (40.11)$$

where $K = 0, 1, 2, \dots$ is a global d -dimensional angular momentum. In particular, at $d = 4$ the hyperspherical harmonic $Y(\theta_i)$ is a product of three factors depending on angles α, β and γ . Two of them are trivial and equal to $e^{im_1\alpha}/\sqrt{2\pi}$ and $e^{im_2\gamma}/\sqrt{2\pi}$, i.e.,

$$Y(\alpha\beta\gamma) = \frac{1}{2\pi} e^{im_1\alpha} \Theta(\beta) e^{im_2\gamma}, \quad m_1, m_2 = 0, \pm 1, \pm 2, \dots \quad (40.12)$$

The β -depending factor satisfies the equation

$$\left(\frac{\partial^2}{\partial \beta^2} + (\cot \beta - \tan \beta) \frac{\partial}{\partial \beta} - \frac{m_1^2}{\sin^2 \beta} - \frac{m_2^2}{\cos^2 \beta} \right) \Theta(\beta) = \lambda \Theta(\beta). \quad (40.13)$$

In this case the spectrum of eigenvalues is given by the formula [1]

$$\lambda = -K(K+2), \quad (40.14)$$

where the four-dimensional (global) angular momentum takes values

$$K = |m_1| + |m_2|, \quad |m_1| + |m_2| + 2, \dots \quad (40.15)$$

The corresponding eigenfunction is of the form [1]

$$\Theta_{Km_1m_2} = Q_{Km_1m_2} \sin^{|m_1|} \beta \cos^{|m_2|} \beta P_{(K-|m_1|-|m_2|)/2}^{(|m_1|, |m_2|)}(\cos 2\beta), \quad (40.16)$$

where $P_n^{(a,b)}(z)$ is the Jacobi polynomial [2].

The normalization factor

$$\begin{aligned} Q_{Km_1m_2} &= \left\{ \left[(2K+2) \left(\frac{K-|m_1|-|m_2|}{2} \right)! \left(\frac{K+|m_1|+|m_2|}{2} \right)! \right]^{1/2} \right. \\ &\times \left. \left\{ \left[\left(\frac{K+|m_1|-|m_2|}{2} \right)! \left(\frac{K-|m_1|+|m_2|}{2} \right)! \right]^{-1/2} \right\} \right\} \end{aligned} \quad (40.17)$$

is chosen so that the following normalization condition for the four-dimensional spherical harmonics is valid:

$$\int d\Omega Y_{Km_1m_2}^*(\Omega)Y_{K'm'_1m'_2}(\Omega) = \delta_{KK'}\delta_{m_1m'_1}\delta_{m_2m'_2}. \quad (40.18)$$

Here,

$$\begin{aligned} Y_{Km_1m_2}(\Omega) &\equiv Y_{Km_1m_2}(\alpha\beta\gamma) \\ &= \frac{1}{2\pi} e^{im_1\alpha} \Theta_{Km_1m_2}(\beta) e^{im_2\gamma}, \end{aligned} \quad (40.19a)$$

$$d\Omega = \sin\beta \cos\beta d\alpha d\beta d\gamma. \quad (40.19b)$$

Taking account the relations (40.8) and (40.11) we can write the differential equation for the radial function of d -dimensional harmonic oscillator in the form

$$\begin{aligned} \frac{1}{2} \left(-\frac{1}{\rho^{d-1}} \frac{\partial}{\partial\rho} \left(\rho^{d-1} \frac{\partial}{\partial\rho} \right) + \frac{K(K+d-2)}{\rho^2} + \rho^2 \right) R(\rho) \\ = ER(\rho). \end{aligned} \quad (40.20)$$

This equation can be solved similarly to Eq. (1.3). As a result we obtain eigenvalues

$$E_{nK} = 2n + K + \frac{d}{2} \quad (40.21)$$

(cf. with Eq. (1.7)) and eigenfunctions

$$R_{nK}(\rho) = N_{nK} \rho^K L_n^{K+(d-2)/2}(\rho^2) e^{-\rho^2/2}, \quad (40.22)$$

where

$$L_n^\alpha(x) = \sum_{k=0}^n \frac{(-1)^k \Gamma(n+\alpha+1)}{k!(n-k)! \Gamma(k+\alpha+1)} x^k \quad (40.23)$$

is an associate Laguerre polynomial [2].

The normalization factor

$$N_{nK} = \left[\frac{2\Gamma(n+1)}{\Gamma(n+K+d/2)} \right]^{1/2} \quad (40.24)$$

is chosen to satisfy the condition

$$\int_0^\infty \rho^{d-1} d\rho R_{nK}(\rho) R_{n'K}(\rho) = \delta_{nn'}. \quad (40.25)$$

Now let us turn to the particular case $d = 4$. Introducing the creation and annihilation operators for the FDHO

$$\begin{aligned} \eta_k &= \frac{1}{\sqrt{2}} \left(x_k - \frac{\partial}{\partial x_k} \right), \\ \xi_k &= \frac{1}{\sqrt{2}} \left(x_k + \frac{\partial}{\partial x_k} \right), \quad k = 1, 2, \dots, d, \end{aligned} \quad (40.26)$$

we can rewrite the eigenfunction of FDHO in the form

$$\Psi_{nKm_1m_2}(\rho, \Omega) = A_{nK} (\eta \cdot \eta)^n \mathcal{Y}_{Km_1m_2}(\eta) |0\rangle, \quad (40.27)$$

similar to the expression (8.16). Here

$$\begin{aligned} A_{nK} &= \left[\frac{2\pi(2K+d-2)!!}{(2n)!!(2K)!!(2n+2K+d-2)!!} \right. \\ &\times \left. \prod_{s=3}^d \left\{ \frac{\sqrt{\pi}\Gamma(K+(s-1)/2)}{\Gamma(K+s/2)} \right\} \right]^{1/2} (-1)^n, \end{aligned} \quad (40.28a)$$

and the scalar product of the four-dimensional vectors is defined in usual manner

$$(\eta \cdot \eta) = \sum_{k=1}^4 \eta_k \eta_k, \quad (40.28b)$$

and the operator expression $\mathcal{Y}_{Km_1m_2}(\eta)$ is obtained from the function $\rho^K Y_{Km_1m_2}(\Omega)$ by substitution $x_k \rightarrow \eta_k$ ($k = 1, 2, 3, 4$). Also the solution of the Schroedinger equation (40.4) in variables ρ_1, ρ_2, α and γ can be found. These coordinates correspond to the presentation of the FDHO Hamiltonian as a sum of a pair of two-dimensional oscillator Hamiltonians $H^{\text{osc}} = H_{12}^{\text{osc}} + H_{34}^{\text{osc}}$. Each of these oscillators is considered in cylindrical coordinates. The solutions of the Schroedinger equation for a two-dimension oscillator,

$$H_{ij}^{\text{osc}} \Psi_{n_{ij}m_{ij}}(x_i, x_j) = E_{n_{ij}m_{ij}} \Psi_{n_{ij}m_{ij}}(x_i, x_j), \quad (40.29)$$

are well known. In accordance with (40.21) the energy eigenvalues are equal to

$$E_{n_{ij}m_{ij}} = 2n_{ij} + |m_{ij}| + 1, \quad (40.30)$$

where

$$m_{ij} = 0, \pm 1, \pm 2, \dots, \quad n_{ij} = 0, 1, 2, \dots \quad (40.31)$$

Corresponding eigenfunctions are of the form

$$\Psi_{n_{ij}m_{ij}}(x_i, x_j) = R_{n_{ij}|m_{ij}|}(\rho_{ij}) \frac{1}{\sqrt{2\pi}} e^{im_{ij}\varphi_{ij}} \quad (40.32)$$

in cylindrical coordinates $x_i = \rho_{ij} \cos \varphi_{ij}$, $x_j = \rho_{ij} \sin \varphi_{ij}$, $\rho_{ij}^2 = x_i^2 + x_j^2$. The radial function is given by the expression

$$R_{n|m|}(\rho) = \sqrt{\frac{2n!}{\Gamma(n+|m|+1)}} \rho^{|m|} L_n^{|m|}(\rho^2) e^{-\rho^2/2}. \quad (40.33)$$

It satisfies the normalization condition

$$\int_0^\infty \rho d\rho R_{n|m|}(\rho) R_{n'|m'|}(\rho) = \delta_{nn'}. \quad (40.34)$$

Taking account all these facts we can write the eigenfunction of the FDHO, corresponding to the energy eigenvalue

$$E_{n_1 n_2 |m_1||m_2|} = 2n_1 + 2n_2 + |m_1| + |m_2| + 2 \quad (40.35)$$

in the form

$$\Psi_{n_1 n_2 m_1 m_2} = \frac{1}{2\pi} R_{n_1|m_1|}(\rho_1) R_{n_2|m_2|}(\rho_2) e^{im_1\alpha} e^{im_2\gamma}, \quad (40.36)$$

where both radial factors are given by the expression (40.33). It is clear that a set of eigenfunctions (40.27) with fixed values of m_1 , m_2 and energy $E_{nK} = (2n + K + 2)$ can be expanded in terms of eigenfunctions (40.36) with the same values of m_1 , m_2 and energy $2n_1 + 2n_2 + |m_1| + |m_2| = 2n + K$:

$$\Psi_{nK m_1 m_2}(\rho, \Omega) = \sum_{n_1 n_2} \langle n_1 m_1 n_2 m_2 | nK m_1 m_2 \rangle \Psi_{n_1 m_1 n_2 m_2}(\rho_1, \rho_2, \alpha, \gamma). \quad (40.37)$$

The transformation bracket $\langle n_1 m_1 n_2 m_2 | nK m_1 m_2 \rangle$ can be found by direct calculation of the integral

$$\int \rho^3 d\rho \sin \beta \cos \beta d\beta R_{nK}(\rho) \Theta_{K m_1 m_2}(\beta) R_{n_1|m_1|}(\rho_1) R_{n_2|m_2|}(\rho_2). \quad (40.38)$$

It can be expressed in terms of the Clebsch–Gordan coefficient for the $\text{sp}(2, R) \simeq \text{su}(1,1)$ algebra [3]:

$$\langle n_1 m_1 n_2 m_2 | nK m_1 m_2 \rangle = (k_1 \mu_1 k_2 \mu_2 | k \mu)_{SU(1,1)}, \quad (40.39)$$

where

$$\begin{aligned} k_1 &= \frac{1}{2}(|m_1| + 1), \quad k_2 = \frac{1}{2}(|m_2| + 1), \quad k = \frac{1}{2}K + 1, \\ \mu_1 &= n_1 + \frac{|m_1| + 1}{2}, \quad \mu_2 = n_2 + \frac{|m_2| + 1}{2}, \quad \mu = n + \frac{K+2}{2}. \end{aligned} \quad (40.40)$$

41 From the Four-Dimension Harmonic Oscillator to the Three-Dimension Coulomb Problem

a) Spherical coordinates

The transition from the FDHO problem to the three-dimensional Coulomb (TDC) problem can be done using the so called Kustaanheimo–Stiefel (KS) transformation [4,5]. It is a nonbijective and nonlinear mapping of the four-dimensional space $R_4(x_1 x_2 x_3 x_4)$ onto the three-dimensional space $R_3(u_1 u_2 u_3)$. In the Cartesian coordinates the KS transformation is of the form

$$\begin{aligned} u_1 &= 2(x_1 x_3 - x_2 x_4), \\ u_2 &= 2(x_1 x_4 + x_2 x_3), \\ u_3 &= x_1^2 + x_2^2 - x_3^2 - x_4^2 \end{aligned} \quad (41.1)$$

at the additional condition

$$\mathcal{O}\psi = \left(x_3 \frac{\partial}{\partial x_4} - x_4 \frac{\partial}{\partial x_3} + x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} \right) \psi = 0. \quad (41.2)$$

If the following hyperspherical coordinates are used in the space R_4 :

$$\begin{aligned} x_1 &= \rho \cos(\theta/2) \cos((\phi + \varphi)/2), \\ x_2 &= \rho \cos(\theta/2) \sin((\phi + \varphi)/2), \\ x_3 &= \rho \sin(\theta/2) \cos((\phi - \varphi)/2), \\ x_4 &= \rho \sin(\theta/2) \sin((\phi - \varphi)/2), \end{aligned} \quad (41.3)$$

i.e., in the expressions (40.7) $\beta = \theta/2$, $\alpha = (\phi + \varphi)/2$, $\gamma = (\phi - \varphi)/2$, $0 \leq \phi \leq 2\pi$, $0 \leq \varphi \leq 4\pi$, the transformation (41.1) corresponds to the introduction of standard spherical coordinates in R_3 :

$$\begin{aligned} u_1 &= r \sin \theta \cos \phi, \\ u_2 &= r \sin \theta \sin \phi, \\ u_3 &= r \cos \theta, \end{aligned} \quad (41.4)$$

where

$$r = (u_1^2 + u_2^2 + u_3^2)^{1/2} = \rho^2. \quad (41.5)$$

After this substitution the radial equation for the FDHO

$$\left[\frac{1}{\rho^3} \frac{\partial}{\partial \rho} \left(\rho^3 \frac{\partial}{\partial \rho} \right) - \frac{K(K+2)}{\rho^2} + \rho^2 + 2E_{nK} \right] R_{nK}(\rho) = 0 \quad (41.6)$$

takes the form

$$\left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{l(l+1)}{r^2} + \frac{2E_{nK}}{4r} - \frac{1}{4} \right] R_{nl}(r) = 0, \quad (41.7)$$

where $K = 2l$.

As for the angular part of the four-dimensional Laplace operator (40.9), it transforms into the expression

$$\begin{aligned} \Delta_\Omega = & \frac{4}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\cos^2(\theta/2)} \left(\frac{\partial}{\partial \phi} - \frac{\partial}{\partial \varphi} \right)^2 \\ & + \frac{1}{\sin^2(\theta/2)} \left(\frac{\partial}{\partial \phi} + \frac{\partial}{\partial \varphi} \right)^2. \end{aligned} \quad (41.8)$$

Its eigenfunctions, corresponding to the eigenvalue $-K(K+2)$, are hyperspherical harmonics (40.16). For example at $m_1, m_2 \geq 0$ we have

$$\begin{aligned} Y_{Km_1m_2}(\theta, \phi, \varphi) \sim & \sin^{m_1}(\theta/2) \cos^{m_2}(\theta/2) P_{(K-m_1-m_2)/2}^{(m_1, m_2)}(\cos \theta) \\ & e^{i(m_1+m_2)\phi/2} e^{i(m_1-m_2)\varphi/2}. \end{aligned} \quad (41.9)$$

In the variables (41.3) the operator \mathcal{O} takes the form

$$\mathcal{O} = \frac{\partial}{\partial \varphi}. \quad (41.10)$$

The constraint condition (41.2) means that we are restricting ourselves to eigenfunctions which do not depend on the angle φ . It means that we select the FDHO wave functions with $m_1 = m_2$ and even values of $K = 2l$ ($l = 0, 1, 2, \dots$) (see Eq. (40.15)) and apply the KS transformation to them. In such a case the expression (41.8) takes the form

$$\frac{1}{4} \Delta_\Omega = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}, \quad (41.11)$$

which coincides with an angular part of the three-dimensional Laplace operator. Since at $m_1 = m_2 = m$ the Jacobi polynomial is connected with the associate Legendre polynomial [2]

$$(1-z^2)^{m/2} P_{l-m}^{m,m}(z) = \frac{2^m l!}{(l+m)!} P_l^m(z), \quad (41.12)$$

the four-dimensional spherical harmonic (41.9) transforms under the KS transformation into usual three-dimensional spherical harmonic

$$Y_{Kmm}(\theta, \phi, \varphi) = \sqrt{\frac{2}{\pi}} Y_{l m}(\theta, \phi), \quad l = K/2, \quad (41.13)$$

as it should be in accordance with (41.11). Thus if we select the FDHO eigenfunctions

$$|nKmm\rangle = R_{nK}(\rho) Y_{Kmm}(\theta, \phi, \varphi), \quad K = \text{even}, \quad (41.14)$$

where

$$R_{nK}(\rho) = \sqrt{\frac{2n!}{(n+K+1)!}} \rho^K e^{-\rho^2/2} L_n^{(K+1)}(\rho^2), \quad (41.15)$$

they transform under KS transformation as a whole into the three-dimensional functions

$$\langle r | nlm \rangle = R_{nl}(r) Y_{lm}(\theta, \phi), \quad l = K/2, \quad (41.16)$$

with radial dependence

$$R_{nl}(r) = \sqrt{\frac{2n!}{(n+2l+1)!}} r^l e^{-r^2/2} L_n^{(2l+1)}(r). \quad (41.17)$$

They satisfy the equation

$$\left(-\Delta - \frac{\nu}{r} \right) |nlm\rangle = -\frac{1}{4} |nlm\rangle, \quad (41.18)$$

where

$$\nu = \frac{1}{2} E_{nK} = (n+l+1). \quad (41.19)$$

The orthonormality condition

$$\int R_{nK}(\rho) R_{n'K}(\rho) \rho^3 d\rho = \delta_{nn'} \quad (41.20)$$

for the functions (40.22) transforms into the following orthonormality relations for the functions (41.16):

$$\frac{1}{2} \int R_{nK}(r) R_{n'K}(r) r dr = \delta_{nn'}. \quad (41.21)$$

Thus the KS transformation reduces the FDHO problem not to the Schrödinger problem for the three-dimensional Coulomb system, but to the Sturmian problem for the three-dimensional Coulomb system (or to the pseudo-Coulomb problem in terms of ref. [6]). In a standard Schrödinger problem the potential $-Z_{eff}/r$ in the Hamiltonian is fixed and the energies $E_{nl}(Z_{eff}) = -1/2\nu^2$ of bound states are quantized ($\nu = n + l + 1$). In a Sturm problem the energy eigenvalue is fixed (in our case $E_{nl} = -1/8$), but the effective charge (or the amplitude of the attractive Coulomb potential) is quantized $Z_{eff} = -\nu$. This difference in formulations of the problems for the Coulomb system is an origin of difference between Sturm–Laguerre eigenfunctions (41.17) (containing the independent of n argument r of both exponent and Laguerre polynomial) and the standard hydrogen-like eigenfunctions which can be obtained from (41.17) by the substitution $r \rightarrow 2r/\nu$. It is also a reason of difference between the orthonormality relation (41.21) for Sturm–Laguerre functions (they are normalized with a volume element $V(r)r^2 dr \sim r dr$ for the Coulomb potential $V(r)$) and the orthonormality relation for the hydrogenlike functions including usual volume element $r^2 dr$.

The standard Schrödinger equation for the hydrogen atom can be obtained from Eq. (41.18) by the substitution $r = 2r/\nu$ mentioned above. As a result we have the equation

$$\left(-\frac{1}{2}\Delta_r - \frac{1}{r}\right)\langle r|nlm\rangle = -\frac{1}{2\nu^2}\langle r|nlm\rangle, \quad (41.22)$$

where $\nu = (n + l + 1)$. In accordance with (41.16) the hydrogen atom eigenfunctions are of the form

$$\langle r|nlm\rangle = R_{nl}^{Coul}(r)Y_{lm}(\hat{r}), \quad (41.23)$$

$$R_{nl}^{Coul}(r) = \frac{1}{N_{nl}}r^l e^{-r/(n+l+1)} L_n^{2l+1}(2r/(n+l+1)). \quad (41.24)$$

The normalization factor N_{nl} should be chosen so that the usual normalization condition satisfies

$$\int_0^\infty R_{nl}^{Coul}(r) R_{n'l'}^{Coul}(r) r^2 dr = \delta_{nn'} \quad (41.25)$$

instead of the relation (41.21).

Thus the transformation of the eigenfunctions of the Sturm–Coulomb problem into hydrogen like eigenfunctions includes two steps: 1) a change of normalization factor, 2) the substitution $r \rightarrow 2r/\nu$ ($\nu = n + l + 1$ in the three-dimension variables or $\rho \rightarrow \rho\sqrt{2/\nu}$) in the four-dimension variable.

The first step is connected with the fact that the hydrogen eigenfunctions are normalized by the condition (41.25) and the Sturm–Coulomb eigenfunctions are normalized with a volume element $r dr$ (see (41.21)). In this connection it is reasonable to change the normalization factor of Sturmian eigenfunctions

$$\tilde{R}_{nl}^{Sturm}(r) = N_\nu^{-1} R_{nl}^{Sturm}(r) \quad (41.26)$$

in order to satisfy the condition

$$\int \tilde{R}_{nl}^{Sturm}(r) \tilde{R}_{n'l'}^{Sturm}(r) r^2 dr = 1. \quad (41.27)$$

It is clear from Eqs. (41.21) and (41.25) that

$$N_\nu^2 = \int R_{nl}^{Sturm}(r) r R_{n'l'}^{Sturm}(r) r dr. \quad (41.28)$$

Using the KS transformation we can write

$$\begin{aligned} N_\nu^2 &= 2 \langle nKm_1m_2 | \rho^2 | nKm_1m_2 \rangle \\ &= 2(2n + K + 2) = 4(n + l + 1) = 4\nu. \end{aligned} \quad (41.29)$$

Thus the renormalization factor is found and we have

$$\tilde{R}_{nl}^{Sturm}(r) = \sqrt{\frac{n!}{2(n+l+1)(n+2l+1)!}} r^l L_n^{2l+1}(r) e^{-r}. \quad (41.30)$$

Now we are doing the rescaling $r \rightarrow 2r/\nu$ using the dilatation operator $D_3(2/\nu)$ which acts on the radial functions $f(r)$ in a three-dimensional space as follows:

$$D_3(a)f(r) = a^{3/2}f(ar). \quad (41.31)$$

As a result we obtain the radial function of the Coulomb problem [7]:

$$\begin{aligned} R_{nl}^{Coul}(r) &= D_3(2/\nu) \cdot \tilde{R}_{nl}^{Sturm}(r) \\ &= \sqrt{\frac{n!}{(n+2l+1)!}} \frac{2^{l+1}}{\nu^2} \left(\frac{r}{\nu}\right)^l L_n^{(2l+1)}\left(\frac{2r}{\nu}\right) e^{-r/\nu}. \end{aligned} \quad (41.32)$$

The explicit form of the dilatation operator $D_d(a)$, acting in a space of any dimension d , is discussed below.

The wave function (41.32) are normalized in correspondence with the condition

$$\int_0^\infty R_{nl}^{\text{Coul}}(r)R_{nl}^{\text{Coul}}(r)r^2 dr = 1. \quad (41.33)$$

These eigenfunctions with different values of the principal quantum number ν are orthogonal:

$$\int_0^\infty R_{n'l}^{\text{Coul}}(r)R_{nl}^{\text{Coul}}(r)r^2 dr = \delta_{nn'}, \quad (41.34)$$

as can be proved in the standard way using Eq. (41.22).

b) Dilatation operator

The dilatation operator, acting in a d -dimensional space of variables x_1, x_2, \dots, x_d , can be written as follows:

$$D_d(a) = \exp \left[-\frac{\tau}{4} \sum_{s=1}^d \left(x_s \frac{\partial}{\partial x_s} + \frac{\partial}{\partial x_s} x_s \right) \right] \quad (41.35a)$$

$$= \exp \left[-\frac{\tau}{2} \left(\sum_{s=1}^d x_s \frac{\partial}{\partial x_s} + \frac{d}{2} \right) \right] \quad (41.35b)$$

$$= a^{(\rho\partial/\partial\rho+d/2)} \quad (41.35c)$$

$$= \exp(-i\tau T_2). \quad (41.35d)$$

Here

$$a = e^{-\tau/2} \text{ or } \tau = -2\ln a, \quad (41.36)$$

and the radial variable ρ is the same as in Eq. (40.5).

It is clear from the expressions (41.35b) or (41.35c) that this operator, acting on some function $\psi(x_1 x_2, \dots, x_d) \equiv \psi(\rho, \theta_1, \theta_2, \dots, \theta_{d-1})$, gives the result

$$D_d(a)\psi(x_1 x_2, \dots, x_d) = a^{d/2}\psi(ax_1 ax_2, \dots, ax_d), \quad (41.37a)$$

or

$$D_d(a)\psi(\rho, \theta_1, \theta_2, \dots, \theta_{d-1}) = a^{d/2}\psi(a\rho, \theta_1, \theta_2, \dots, \theta_{d-1}). \quad (41.37b)$$

Thus this operator changes a linear scale in the d -dimensional space and can be considered as the dilatation operator.

The expression (41.35d) contains the operator

$$T_2 = -\frac{i}{4} \sum_{s=1}^d \left(x_s \frac{\partial}{\partial x_s} + \frac{\partial}{\partial x_s} x_s \right) \quad (41.38a)$$

$$= -\frac{i}{2} \left(\sum_{s=1}^d x_s \frac{\partial}{\partial x_s} + \frac{d}{2} \right) \quad (41.38b)$$

$$= -\frac{i}{4} \sum_{s=1}^d (\eta_s \eta_s - \xi_s \xi_s), \quad (41.38c)$$

which is a generator of the $\text{sp}(2, R)$ algebra. In fact it is a d -dimensional generalization of the generator (34.18).

The two other generators of this algebra are of the form

$$T_3 = \frac{1}{2} \left(\sum_{s=1}^d \eta_s \xi_s + \frac{d}{2} \right), \quad (41.39a)$$

$$T_1 = -\frac{1}{4} \sum_{s=1}^d (\eta_s \eta_s + \xi_s \xi_s), \quad (41.39b)$$

or

$$T_+ = T_1 + iT_2 = -\frac{1}{2} \sum_{s=1}^d \eta_s \eta_s, \quad (41.40a)$$

$$T_- = T_1 - iT_2 = -\frac{1}{2} \sum_{s=1}^d \xi_s \xi_s. \quad (41.40b)$$

They satisfy the same commutation relations (34.15) and (34.19) which were obtained in the Chapter VII for the one-dimensional case.

The dilatation operator (41.35d), containing the $\text{sp}(2, R)$ generator T_2 in the exponent, is an element of the group of canonical transformations $\text{Sp}(2, R)$. It is a unitary one, i.e.,

$$[D_d(a)]^\dagger = D_d \left(\frac{1}{a} \right) = D_d^{-1}(a), \quad (41.41)$$

and produces the following transformation of coordinates x_s and momenta $p_s = -i\partial/\partial x_s$:

$$D_d(e^{-\tau/2}) x_s D_d^{-1}(e^{-\tau/2}) = e^{-\tau/2} x_s, \quad (41.42)$$

$$D_d(e^{-\tau/2}) p_s D_d^{-1}(e^{-\tau/2}) = e^{\tau/2} p_s, \quad (41.43)$$

where the last equation follows immediately from relation (40.2). It should be noted that radial wave functions (40.22) of the d -dimensional harmonic oscillator with fixed global angular momentum K ($n = 0, 1, 2, \dots$) form a basis of an infinite-dimensional irreducible representation D^k , belonging to

the positive discrete series of the unitary irreducible representation of the algebra $\text{sp}(2, R)$ (and the corresponding noncompact group $\text{Sp}(2, R)$).

The functions (40.22) can be characterized by a definite weight μ that is an eigenvalue of the T_3 generator:

$$\mu = \frac{1}{2} E_{nK} = \frac{1}{2} \left(2n + K + \frac{d}{2} \right). \quad (41.44)$$

The signature k of the $\text{Sp}(2, R)$ irreducible representation D^k coincides with the lowest weight, i.e., with a minimal value of μ :

$$k = \frac{1}{2} E_{0K} = \frac{1}{2} \left(K + \frac{d}{2} \right). \quad (41.45)$$

For brevity we call k and μ a “noncompact” spin and its projection respectively.

Thus the wave functions (40.22) can be considered as standard basis vectors

$$|k\mu\rangle \equiv R_{nK}(\rho), \quad \mu = k, k+1, \dots \quad (41.46)$$

of the $\text{Sp}(2, R)$ irreducible representation D^k , corresponding to the non-compact spin and its projection, given by Eqs. (41.44) and (41.45).

It is clear from the relations (41.37) and (41.42) that the dilatation operator $D_d(e^{-\tau/2})$ transforms the normalized function (40.22) of unit frequency $\omega = 1$ into the normalized harmonic oscillator function of frequency $\omega' = e^{-\tau}$ with the same quantum numbers n and K :

$$D_d(e^{-\tau/2}) R_{nK}(\rho; \omega = 1) = R_{nK}(\rho; \omega' = e^{-\tau}). \quad (41.47)$$

The last one can be expanded in terms of the harmonic oscillator functions of the initial frequency $\omega = 1$ (with the same value of K):

$$D_d(e^{-\tau/2}) R_{nK}(\rho) = \sum_{n'} C_{n'n}^K(\tau) R_{n'K}(\rho). \quad (41.48)$$

The coefficient of this expansion can be calculated as follows:

$$C_{n'n}^K(\tau) \equiv \int \rho^{d-1} d\rho R_{n'K}(\rho; \omega = 1) R_{nK}(\rho, \omega' = e^{-\tau}) \quad (41.49a)$$

$$= \langle R_{n'K} | D_d(e^{-\tau/2}) | R_{nK} \rangle \quad (41.49b)$$

$$= \langle k\mu' | e^{i\tau T_2} | k\mu \rangle \quad (41.49c)$$

$$\equiv d_{\mu'\mu}^k(\tau), \quad (41.49d)$$

and this coefficient can be considered in the following ways: 1) as an overlap integral (41.49a) of two radial harmonic oscillator functions, corresponding to different frequencies ω and ω' ; 2) as a matrix element of the dilatation operator (41.49b) in the harmonic oscillator basis; 3) as a matrix element of boost (41.49c) which coincides with a d -function (41.49d) for the D^k irreducible representation of the group $\text{Sp}(2, R) \approx \text{SU}(1, 1)$.

This d -function can be taken from ref. [1]:

$$d_{\mu\mu'}^k(\tau) = (-1)^{\mu'-\mu} \sqrt{(k+\mu-1)!(k+\mu'-1)!(\mu-k)!(\mu'-k)!} \\ \times \frac{(\sinh \frac{\tau}{2})^{\mu'-\mu}}{(\cosh \frac{\tau}{2})^{\mu+\mu'}} \sum_{y=0}^{\infty} \frac{(-1)^y (\sinh^2 \frac{\tau}{2})^y}{y!(\mu'-\mu+y)!(\mu+k-1-y)!(\mu-k-y)!}. \quad (41.50)$$

Also the coefficient $C_{n'n}^K(\tau)$ were calculated in refs. [6,8].

The isotropic dilatation-squeezing in the d -dimensional space was discussed above. However the operators (41.35) can be used also in order to obtain anisotropic oscillator wave functions from the isotropic oscillator ones. For example the wave function of the deformed three-dimensional harmonic oscillator with frequencies $\omega_x, \omega_y, \omega_z$ can be obtained from the isotropic oscillator wave function of the frequency ω_0 (in Cartesian coordinates) as follows:

$$|n_x n_y n_z; \omega_x \omega_y \omega_z\rangle = D_1(a_x) D_1(a_y) D_1(a_z) |n_x n_y n_z; \omega_0\rangle. \quad (41.51)$$

Here $a_i = \sqrt{\omega_i/\omega_0}$, $i = x, y, z$.

The relation (41.51) can be used for the investigation of the properties of deformed nuclei in a frame of the unified nuclear model. However our aim in this Section is a mapping of the FDHO wave functions onto wave functions of the Coulomb problem. In the subsection 41.a it was done by KS transformation for the case of spherical coordinates. Now we map the FDHO wave functions (40.36) onto Coulomb wave functions in parabolic coordinates s_1, s_2, ϕ , connected with variables (41.4) by the relations

$$u_1 = \sqrt{s_1 s_2} \cos \phi, \quad u_2 = \sqrt{s_1 s_2} \sin \phi, \\ u_3 = (s_1 - s_2)/\frac{1}{2}, \quad r = (s_1 + s_2)/2. \quad (41.52)$$

c) Parabolic coordinates

It is known [7] that the Coulomb wave functions are given in parabolic coordinates by the following expression:

$$\begin{aligned} \Psi_{n_1 n_2 m}(s_1, s_2, \phi) &= \sqrt{\frac{2n_1! n_2!}{(n_1 + |m|)! (n_2 + |m|)!}} \frac{1}{\nu^2} \left(\frac{s_1 s_2}{\nu^2}\right)^{|m|/2} L_{n_1}^{|m|} \left(\frac{s_1}{\nu}\right) \\ &\times L_{n_2}^{|m|} \left(\frac{s_2}{\nu}\right) e^{-(s_1 + s_2)/2\nu} \frac{1}{\sqrt{2\pi}} e^{im\phi}, \end{aligned} \quad (41.53)$$

where

$$\nu = n_1 + n_2 + |m| + 1, \quad n_1, n_2 = 0, 1, 2, \dots$$

They are normalized in correspondence with the condition

$$\begin{aligned} \frac{1}{4} \int_0^\infty ds_1 \int_0^\infty ds_2 \int_0^{2\pi} d\phi (s_1 + s_2) \Psi_{n'_1 n'_2 m'}^*(s_1, s_2, \phi) \Psi_{n_1 n_2 m}(s_1, s_2, \phi) \\ = \delta_{n_1 n'_1} \delta_{n_2 n'_2} \delta_{mm'}. \end{aligned} \quad (41.54)$$

In order to transform the wave function (40.36) $\Psi_{n_1 n_2 mm}$ into the functions (41.53) it is necessary to do the following steps:

1. To do the rescaling $\rho_1 \rightarrow \rho_1/\sqrt{\nu}$, $\rho_2 \rightarrow \rho_2/\sqrt{\nu}$ using the dilatation operator $D_4(1/\sqrt{\nu})$ in the fourdimensional space, which can be expressed in terms of the dilatation operators, acting in two-dimensional spaces of variables x_1 , x_2 and x_3 , x_4 respectively:

$$D_4 \left(\frac{1}{\sqrt{\nu}} \right) = D_2^{12} \left(\frac{1}{\sqrt{\nu}} \right) D_2^{34} \left(\frac{1}{\sqrt{\nu}} \right). \quad (41.55)$$

2. Do the substitutions

$$\rho_1^2 = s_1, \quad \rho_2^2 = s_2. \quad (41.56)$$

3. To complete the normalization factor in (40.36) by additional factor $\nu(\sqrt{2})^{-1}$ in order to satisfy the normalization condition (41.54).

In other words, if we take the FDHO wave function of the form

$$\frac{1}{\nu\sqrt{2}} D_4 \left(\frac{1}{\sqrt{\nu}} \right) \Psi_{n_1 n_2 mm}(\rho_1, \rho_2, \alpha, \gamma), \quad (41.57)$$

it coincides with (41.53), multiplied by the factor $1/\sqrt{4\pi}$, after the substitution (41.56) and remembering the definition of α and γ after (41.3). This fact can be used to find the matrix elements of some multiplicative operator $W(s_1, s_2, \phi)$ between Coulomb wave functions (41.53) calculating the corresponding matrix element of the operator

$$\tilde{W}(\rho_1, \rho_2, \phi) = (\rho_1^2 + \rho_2^2) W(\rho_1^2, \rho_2^2, \phi) \quad (41.58)$$

between the FDHO wave functions (40.36).

Namely,

$$\begin{aligned} &\left\langle D_4 \left(\frac{1}{\sqrt{\nu'}} \right) \Psi_{n'_1 n'_2 m' m'}^*(\rho_1, \rho_2, \phi, \varphi) \mid \tilde{W}(\rho_1, \rho_2, \phi) \right| \\ &\times D_4 \left(\frac{1}{\sqrt{\nu}} \right) \Psi_{n_1 n_2 mm}(\rho_1, \rho_2, \phi, \varphi) \rangle \\ &= \frac{\nu\nu'}{2} \int ds_1 ds_2 d\phi (s_1 + s_2) \Psi_{n'_1 n'_2 m'}^*(s_1, s_2, \phi) \\ &\times W(s_1, s_2, \phi) \Psi_{n_1 n_2 m}(s_1, s_2, \phi). \end{aligned} \quad (41.59)$$

The factors $(1/\sqrt{4\pi})$, mentioned above, cancel after integration on the angle φ from 0 to 4π in the l.h.s. of this relation. The term $(\rho_1^2 + \rho_2^2)$ in Eqs. (41.58) and (41.59) is necessary to reproduce the factor $(s_1 + s_2)$ which is present in a three-dimension volume element for the parabolic coordinates and is absent in the four-dimensional volume element $\rho_1 d\rho_1 \rho_2 d\rho_2 = ds_1 ds_2/4$.

d) Matrix elements of a dipole momentum

As an application of the interrelations between FDHO and Coulomb problem discussed in this chapter we consider the matrix elements of the electric dipole momentum operator

$$\mathbf{d} = e\mathbf{r} \quad (41.60)$$

between the Coulomb eigenfunctions in parabolic coordinates. They are important for the study of electromagnetic transitions and Stark effect in a hydrogen atom. We restrict ourselves to the consideration of the dipole momentum component z .

We are interested in a matrix element

$$\langle n'_1 n'_2 m | z | n_1 n_2 m \rangle = \frac{1}{2} \langle n'_1 n'_2 m | s_1 - s_2 | n_1 n_2 m \rangle. \quad (41.61)$$

In accordance with Eqs. (41.58) and (41.59) we can write

$$\begin{aligned} \langle n'_1 n'_2 m | z | n_1 n_2 m \rangle &= \frac{1}{4\nu\nu'} \langle D_4(1/\sqrt{\nu'}) \psi_{n'_1 n'_2 m'}(\rho_1, \rho_2, \phi, \varphi) | (\rho_1^4 - \rho_2^4) | \\ &\times D_4(1/\sqrt{\nu}) \psi_{n_1 n_2 mm}(\rho_1, \rho_2, \phi, \varphi) \rangle \\ &= \frac{\nu'}{4\nu} \langle \psi_{n'_1 n'_2 m'}(\rho_1, \rho_2, \phi, \varphi) | (\rho_1^4 - \rho_2^4) | \\ &\times D_4(\sqrt{\nu'/\nu}) | \psi_{n_1 n_2 mm}(\rho_1, \rho_2, \phi, \varphi) \rangle \end{aligned}$$

$$\begin{aligned}
&= \frac{\nu'}{4\nu} \left\{ \sum_{n''_1} \langle n'_1 m | \rho_1^4 | n''_1 m \rangle \langle n''_1 m | \right. \\
&\quad \times D_2(\sqrt{\nu'/\nu}) | n_1 m \rangle \langle n'_2 m | D_2(\sqrt{\nu'/\nu}) | n_2 m \rangle \\
&\quad - \sum_{n''_2} \langle n'_2 m | \rho_2^4 | n''_2 m \rangle \langle n'_1 m | \\
&\quad \left. \times D_2(\sqrt{\nu'/\nu}) | n_1 m \rangle \langle n''_2 m | D_2(\sqrt{\nu'/\nu}) | n_2 m \rangle \right\}. \quad (41.62)
\end{aligned}$$

The matrix elements of ρ_1^4 and ρ_2^4 can be calculated using the matrix elements of ρ^2 in two-dimension harmonic oscillator basis

$$\begin{aligned}
\langle R_{n+1|m|}(\rho) | \rho^2 | R_{n|m|}(\rho) \rangle &= -\sqrt{(n+1)(n+|m|+1)}, \\
\langle R_{n|m|}(\rho) | \rho^2 | R_{n|m|}(\rho) \rangle &= 2n + |m| + 1, \\
\langle R_{n-1|m|}(\rho) | \rho^2 | R_{n|m|}(\rho) \rangle &= -\sqrt{n(n+|m|)}. \quad (41.63)
\end{aligned}$$

The matrix elements of the dilatation operator can be found using the formula (41.50) (see also refs. [7,9]). The relations (41.62) and (41.63) allow us to find the matrix elements (41.61) of the dipole momentum operator for the hydrogen atom in a pure algebraic way without calculations of any integrals in an explicit form [7].

42 Dynamic and Invariance Algebras of the Coulomb Problem

Our aim in this section is to find the invariance and dynamic algebras of the Coulomb problem starting from dynamic and invariance algebras for the FDHO, which are known (see Section 37 of the Chapter VII).

The total dynamic algebra of the FDHO is $Sp(8, R)$. If we express its generators in terms of radial and angular (four-dimensional) coordinates and apply them to the eigenvectors of FDHO with $m_1 = m_2$ and $K = 2l = even$, which form the subspace L_r , then the generators, which are proportional to the operator \hat{O} , vanish. The rest of the generators simplify because of the annulation of terms containing $\partial/\partial\varphi$.

As a result the $Sp(8, R)$ algebra, acting in the subspace L_r of such vectors, becomes equivalent to some Lie algebra G of smaller rank and order. This algebra G , which is a subalgebra of $Sp(8, R)$, is called the restriction of the $Sp(8, R)$ algebra by the constraint condition (41.2) [9]. The subalgebra $so(2)$, whose generator is an operator \hat{O} has the name of restricting algebra [9]. It should be noted that the vectors $|\psi\rangle$ of the subspace L_r are invariants of $so(2)$ subalgebra, i.e.,

$$\mathcal{O} |\psi\rangle = \frac{\partial}{\partial\varphi} |\psi\rangle = 0, \quad (42.1)$$

so we go to the concept of the Lie algebra under constraint, introduced in ref. [9]. The essence of this concept is the following: Let us have some Lie algebra \mathfrak{G} and select its subalgebra

$$G \oplus M \in \mathfrak{G}. \quad (42.2)$$

Here $G \oplus M$ is a direct sum of Lie algebras G and M therefore the G and M generators commute.

We consider the irreducible representation D^A of the \mathfrak{G} algebra, which can be expanded in terms of the $G \oplus M$ irreducible representations as follows:

$$D^A = \sum_{a,\mu} D^a \times D^\mu. \quad (42.3)$$

Then only the terms of this expansion, which are invariant with respect to the M subalgebra, which correspond to the unit irreducible representation D^μ with $\mu = 0$, are considered. The subalgebra G will be called the Lie algebra \mathfrak{G} under constraint $\mu = 0$.

In our subspace L_r of the $so(2)$ -invariant vectors the irreducible representations D^A of some restricted algebra G , combining with the unit irreducible representation of $so(2)$, are realized. Evidently our problem of the restriction of the $sp(8, R)$ algebra by the condition (42.1) is a particular case of the Lie algebra under constraint.

In order to establish an explicit form of the G algebra the generators of $sp(8, R)$ commuting with the \mathcal{O} operator should be selected. The simplest way to do it is to use the realization of the $sp(8, R)$ algebra in terms of creation-annihilation operators

$$\eta_i = \frac{1}{\sqrt{2}} \left(x_i - \frac{\partial}{\partial x_i} \right), \quad \xi_i = \frac{1}{\sqrt{2}} \left(x_i + \frac{\partial}{\partial x_i} \right), \quad i = 1, 2, 3, 4. \quad (42.4)$$

As it was mentioned in the Section 37, the total set of bilinear combinations of these operators,

$$\eta_i \eta_k, \quad \xi_i \xi_k \quad \text{and} \quad \frac{1}{2} (\eta_i \xi_k + \xi_k \eta_i), \quad i, k = 1, 2, 3, 4, \quad (42.5)$$

forms a set of the $sp(8, R)$ generators.

For our aims it is more convenient to use instead of Cartesian creation-annihilation operators satisfying the commutation relations

$$[\eta_i, \eta_k] = [\xi_i, \xi_k] = 0, \quad [\xi_i, \eta_k] = \delta_{ik}, \quad (42.6)$$

a new set of creation–annihilation operators:

$$\begin{aligned}\tilde{\eta}_1 &= \frac{1}{\sqrt{2}}(\eta_1 - i\eta_2), & \tilde{\xi}_1 &= \frac{1}{\sqrt{2}}(\xi_1 + i\xi_2), \\ \tilde{\eta}_2 &= \frac{1}{\sqrt{2}}(\eta_1 + i\eta_2), & \tilde{\xi}_2 &= \frac{1}{\sqrt{2}}(\xi_1 - i\xi_2), \\ \tilde{\eta}_3 &= \frac{1}{\sqrt{2}}(\eta_3 - i\eta_4), & \tilde{\xi}_3 &= \frac{1}{\sqrt{2}}(\xi_3 + i\xi_4), \\ \tilde{\eta}_4 &= \frac{1}{\sqrt{2}}(\eta_3 + i\eta_4), & \tilde{\xi}_4 &= \frac{1}{\sqrt{2}}(\xi_3 - i\xi_4).\end{aligned}\quad (42.7)$$

Because of the unitarity of the transformation (42.7) the commutation relations for the operators with a tilde are the same as (42.6):

$$[\tilde{\eta}_i, \tilde{\eta}_k] = [\tilde{\xi}_i, \tilde{\xi}_k] = 0, \quad [\tilde{\xi}_i, \tilde{\eta}_k] = \delta_{ik}. \quad (42.8)$$

In terms of new creation–annihilation operators the generator \mathcal{O} can be expressed as follows:

$$\mathcal{O} = \tilde{\eta}_1 \tilde{\xi}_1 - \tilde{\eta}_2 \tilde{\xi}_2 - \tilde{\eta}_3 \tilde{\xi}_3 + \tilde{\eta}_4 \tilde{\xi}_4 = \tilde{N}_1 - \tilde{N}_2 - \tilde{N}_3 + \tilde{N}_4, \quad (42.9a)$$

where

$$\tilde{N}_i \equiv \tilde{\eta}_i \tilde{\xi}_i \quad (42.9b)$$

is the number of oscillator quanta along i th degree of freedom.

Now it is easy to select the $sp(8, R)$ generators, which commute with \mathcal{O} . As a result we find 16 operators:

$$\begin{aligned}A_{11} &= \tilde{\eta}_1 \tilde{\xi}_1, & A_{12} &= \tilde{\eta}_1 \tilde{\xi}_4, & A_{13} &= \tilde{\eta}_1 \tilde{\eta}_2, & A_{14} &= \tilde{\eta}_1 \tilde{\eta}_3, \\ A_{21} &= \tilde{\eta}_4 \tilde{\xi}_1, & A_{22} &= \tilde{\eta}_4 \tilde{\xi}_4, & A_{23} &= \tilde{\eta}_4 \tilde{\eta}_2, & A_{24} &= \tilde{\eta}_4 \tilde{\eta}_3, \\ A_{31} &= -\tilde{\xi}_2 \tilde{\xi}_1, & A_{32} &= -\tilde{\xi}_2 \tilde{\xi}_4, & A_{33} &= -\tilde{\eta}_2 \tilde{\xi}_2 - 1, & A_{34} &= -\tilde{\eta}_3 \tilde{\xi}_2, \\ A_{41} &= -\tilde{\xi}_3 \tilde{\xi}_1, & A_{42} &= -\tilde{\xi}_3 \tilde{\xi}_4, & A_{43} &= -\tilde{\eta}_2 \tilde{\xi}_3, & A_{44} &= -\tilde{\eta}_3 \tilde{\xi}_3 - 1,\end{aligned}\quad (42.10)$$

which conserve the relation

$$\tilde{N}_1 + \tilde{N}_4 = \tilde{N}_2 + \tilde{N}_3. \quad (42.11)$$

The following commutation relations can be obtained for these operators by direct calculations:

$$[A_{ik}, A_{lm}] = \delta_{kl} A_{im} - \delta_{im} A_{lk}. \quad (42.12)$$

This fact together with the properties of these operators with respect to Hermitian conjugation,

$$A_{ik} = A_{ki}^\dagger \text{ at } i, k = 1, 2 \text{ or } i, k = 3, 4, \quad (42.13)$$

and

$$A_{ik} = -A_{ki}^\dagger \text{ at } i = 1, 2 \text{ and } k = 3, 4, \quad (42.14)$$

mean that the operators A_{ik} are the generators of the noncompact $u(2, 2)$ algebra. After omitting of the \mathcal{O} operator from this set it becomes the basis of the $su(2, 2)$ subalgebra. Thus the role of the $sp(8, R)$ algebra under constraint (41.2) or (42.11) is played by the algebra $G = su(2, 2)$. It is well known that $su(2, 2)$ algebra is isomorphic to the conformal $so(4, 2)$ algebra. A standard basis of $so(4, 2)$ contains 15 generators I_{jk} ($j < k = 1, 2, \dots, 6$) satisfying the commutation relations

$$[I_{ij}, I_{kl}] = \delta_{jk} I_{il} + \delta_{il} I_{jk} - \delta_{jl} I_{ik} - \delta_{ik} I_{jl}. \quad (42.15)$$

The generators I_{jk} ($j < k = 1, 2, 3, 4$) and I_{56} of subalgebras $so(4)$ and $so(2)$ respectively are antihermitian and antisymmetric:

$$(I_{ij})^\dagger = I_{ji} = -I_{ij}, \quad (i, j = 1, 2, 3, 4; i, j = 5, 6). \quad (42.16)$$

The generators I_{ij} ($i = 1, 2, 3, 4, j = 5, 6$) are hermitian and symmetric:

$$I_{ij} = I_{ji} = (I_{ij})^\dagger, \quad (i = 1, 2, 3, 4, j = 5, 6). \quad (42.17)$$

The standard $so(4, 2)$ generators are connected with the Cartan–Weyl generators of $su(2, 2)$ by the relations

$$\begin{aligned}I_{12} &= -\frac{1}{2}(t_{15} + t_{16}), & I_{23} &= \frac{1}{2}(t_5 - t_6), \\ I_{13} &= \frac{1}{2}(t_7 - t_8), & I_{24} &= \frac{i}{2}(t_5 + t_6), \\ I_{14} &= \frac{i}{2}(t_7 + t_8), & I_{25} &= -\frac{1}{2}(t_3 + t_4), \\ I_{15} &= -\frac{1}{2}(t_1 + t_2), & I_{26} &= -\frac{i}{2}(t_3 - t_4), \\ I_{16} &= -\frac{i}{2}(t_1 - t_2), & I_{34} &= -\frac{i}{2}(t_{13} - t_{14}), \\ I_{35} &= \frac{1}{4}(t_9 + t_{10} - t_{11} - t_{12}), \\ I_{36} &= \frac{i}{4}(t_9 - t_{10} - t_{11} + t_{12}), \\ I_{45} &= -\frac{i}{4}(t_9 - t_{10} + t_{11} - t_{12}), \\ I_{46} &= \frac{1}{4}(t_9 + t_{10} + t_{11} + t_{12}), & I_{56} &= \frac{i}{2}(t_{13} + t_{14}).\end{aligned}\quad (42.18)$$

Here

$$t_1 = \xi_1 \xi_3 - \xi_2 \xi_4, \quad t_7 = \eta_1 \xi_3 - \eta_2 \xi_4, \quad t_{13} = \eta_1 \xi_1 + \eta_2 \xi_2 + 1,$$

$$t_2 = \eta_1 \eta_3 - \eta_2 \eta_4, \quad t_8 = \eta_3 \xi_1 - \eta_4 \xi_2, \quad t_{14} = \eta_3 \xi_3 + \eta_4 \xi_4 + 1,$$

$$\begin{aligned} t_3 &= \xi_1\xi_4 + \xi_2\xi_3, \quad t_9 = \xi_1\xi_1 + \xi_2\xi_2, \quad t_{15} = \eta_2\xi_1 - \eta_1\xi_2, \\ t_4 &= \eta_1\eta_4 + \eta_2\eta_3, \quad t_{10} = \eta_1\eta_1 + \eta_2\eta_2, \quad t_{16} = \eta_4\xi_3 - \eta_3\xi_4, \\ t_5 &= \eta_1\xi_4 + \eta_2\xi_3, \quad t_{11} = \xi_3\xi_3 + \xi_4\xi_4, \\ t_6 &= \eta_4\xi_1 + \eta_3\xi_2, \quad t_{12} = \eta_3\eta_3 + \eta_4\eta_4. \end{aligned} \quad (42.19a)$$

The harmonic oscillator Hamiltonian

$$H^{\text{osc}} = -2iI_{56} \quad (42.19b)$$

is proportional to one of the $\text{so}(4, 2)$ generators. Thus $\text{so}(4, 2)$ is the dynamical algebra of the FDHO under constraint. Also it is the dynamic algebra of the Sturm-Coulomb problem because the Schrödinger equation for the FDHO and its eigenfunctions (with $m_1 = m_2$) transform into the Sturm equation for the three-dimensional Coulomb problem and into corresponding eigenfunctions by the KS transformation. Now we apply this type of mapping to some subalgebras of $\text{sp}(8, R)$.

1) $\text{u}(4), \text{su}(4)$. It is a maximal symmetry algebra of the FDHO. It is generated by the operators

$$C_{ij} = \tilde{\eta}_i \tilde{\xi}_j \quad (i, j = 1, 2, 3, 4). \quad (42.20)$$

The transition from $\text{u}(4)$ to $\text{su}(4)$ is reached by omitting the operator of number of quanta:

$$N = \tilde{N}_1 + \tilde{N}_2 + \tilde{N}_3 + \tilde{N}_4 = N_1 + N_2 + N_3 + N_4. \quad (42.21)$$

After taking account the constraint condition (42.9) only the generators I_{ij} (42.18) with $i < j = 2, 3, 4$ survive, forming the algebra $\text{so}_{\text{Coul}}(4) \simeq \text{so}(3) \oplus \text{so}(3)$. It is a maximal symmetry algebra of the Sturm-Coulomb problem. The degenerate FDHO states with fixed value of N form the basis of the symmetric $\text{u}(4)$ irreducible representation $D^{[N]}$. Similarly the degenerate states of the Sturm-Coulomb problem with fixed $\nu = N/2 = n+l+1$ form the basis of the irreducible representation $D^{(\nu, 0)}$ of the $\text{so}_{\text{Coul}}(4)$.

2) $\text{soosc}(4)$. This algebra is the subalgebra of the $\text{u}(4)$ invariance algebra of FDHO. Its generators are of the form

$$\eta_i \xi_j - \eta_j \xi_i, \quad i < j = 2, 3, 4. \quad (42.22)$$

Its irreducible representations are labelled by the global angular momentum K . It transforms under constraint (42.9) into $\text{so}_{\text{Coul}}(3)$ subalgebra with irreducible representations labelled by the angular momentum $l = K/2$. Three generators of $\text{soosc}(4)$ vanish under constraint.

3) $\text{sp}(2, R)$. This dynamic algebra of the FDHO is generated by operators

$$K_+ = \frac{1}{2} \tilde{\eta}_i \tilde{\eta}_i, \quad K_- = \frac{1}{2} \tilde{\xi}_i \tilde{\xi}_i, \quad K_0 = \frac{1}{4} (\tilde{\eta}_i \tilde{\xi}_i + \tilde{\xi}_i \tilde{\eta}_i) \quad (42.23)$$

satisfying the commutation relations

$$[K_0, K_{\pm}] = \pm K_{\pm}, \quad [K_+, K_-] = -2K_0. \quad (42.24)$$

(The summation on repeated indices from 1 to 4 is assumed in (42.21)). By KS transformation the K_{\pm}, K_0 go into the $\text{su}(1, 1)$ algebra with generators

$$\begin{aligned} k_+ &= r \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} + \frac{1}{4} \right] - r \frac{d}{dr} - 1 \\ k_- &= r \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} + \frac{1}{4} \right] + r \frac{d}{dr} + 1 \\ k_0 &= -r \left[\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} \right) - \frac{l(l+1)}{r^2} - \frac{1}{4} \right] \end{aligned} \quad (42.25)$$

satisfying the same commutation relations (42.24). The eigenstates $|nlm\rangle$ with fixed l and m quantum numbers form a basis of the irreducible representation D^k of the $\text{su}(1, 1)$ algebra, which corresponds to the eigenvalue $k(k-1)$ of the Casimir operator

$$C_2(\text{su}(1, 1)) = k_0^2 - k_0 + k_+ k_-. \quad (42.26)$$

The algebras $\text{soosc}(4)$ and $\text{sp}(2, R)$ are complementary ones. Their Casimir operators are connected by the relation

$$C_2(\text{sp}(2, R)) = \frac{1}{4} C_2(\text{soosc}(4)). \quad (42.27)$$

A comparison of their eigenvalues $g_2(\text{sp}(2, R)) = k(k-1)$ and $g_2(\text{soosc}(4)) = K(K+2)$ gives

$$k = \frac{1}{2} K + 1. \quad (42.28)$$

The corresponding algebras under constraint $\text{so}_{\text{Coul}}(3)$ and $\text{su}(1, 1)$ are also complementary ones. Their Casimir operators are connected by the relation

$$C_2(\text{su}(1, 1)) = C_2(\text{so}_{\text{Coul}}(3)). \quad (42.29)$$

The comparison of their eigenvalues $k(k-1)$ and $l(l+1)$ gives

$$k = l + 1, \quad (42.30)$$

which is in correspondence with Eq. (42.28) because $l = K/2$. Thus the states $|nlm\rangle$ with fixed l and m and $n = 0, 1, 2, \dots$ form the basis of the

infinite-dimensional irreducible representation D^{l+1} of $\text{su}(1, 1)$, containing the generator of dilatations in four- and three-dimension spaces respectively:

$$K_2 = -\frac{i}{2} (K_+ - K_-) = \frac{i}{2} \left(\rho \frac{\partial}{\partial \rho} + 2 \right), \quad (42.31)$$

and

$$k_2 = -\frac{i}{2} (k_+ - k_-) = i \left(r \frac{\partial}{\partial r} + 1 \right). \quad (42.32)$$

The operators

$$D(\tau) = e^{-i\tau K_2} \text{ and } d(\tau) = e^{-i\tau k_2} \quad (42.33)$$

are doing the rescaling of the variables ρ and r respectively:

$$D(\tau)\Psi(\rho) = e^{\tau}\Psi\left(e^{\tau/2}\rho\right), \quad (42.34)$$

$$d(\tau)\psi(r) = e^{\tau}\phi(e^{\tau}r). \quad (42.35)$$

These operators are necessary to transform the Sturm–Coulomb eigenfunction to the standard hydrogen-like wave functions of bound states.

The Casimir operator for the $\text{su}(2, 2)$ algebra is of the form

$$\begin{aligned} C_2(\text{u}(2, 2)) = & \tilde{\eta}_4^2 \tilde{\xi}_4^2 - 2\tilde{\eta}_3\tilde{\eta}_4\tilde{\xi}_3\tilde{\xi}_4 - 2\tilde{\eta}_2\tilde{\eta}_4\tilde{\xi}_2\tilde{\xi}_4 + 2\tilde{\eta}_3\tilde{\xi}_3 + 2\tilde{\eta}_2\tilde{\xi}_2 \\ & + \tilde{\eta}_3^2 \tilde{\xi}_3^2 + 2\tilde{\eta}_2\tilde{\eta}_3\tilde{\xi}_2\tilde{\xi}_3 + 2\tilde{\eta}_1\tilde{\eta}_4\tilde{\xi}_1\tilde{\xi}_4 - 2\tilde{\eta}_1\tilde{\eta}_3\tilde{\xi}_1\tilde{\xi}_3 \\ & + \tilde{\eta}_2^2 \tilde{\xi}_2^2 + \tilde{\eta}_1^2 \tilde{\xi}_1^2 - 2\tilde{\eta}_1\tilde{\eta}_2\tilde{\xi}_1\tilde{\xi}_2 - 2. \end{aligned} \quad (42.36)$$

The application of this operator to the lowest weight vector $|000000\rangle$ (the ground state of the FDHO) gives

$$C_2(\text{su}(2, 2))|000000\rangle = -2|000000\rangle. \quad (42.37)$$

The Casimir operator for the $\text{so}(4, 2)$ algebra can be expressed in terms of its generators as follows:

$$C_2(\text{so}(4, 2)) = \sum_{i < j} I_{ij} I_{ji}. \quad (42.38)$$

Using the realization of generators I_{ij} in terms of creation–annihilation operators (see Eqs. (42.18)) we obtain

$$\begin{aligned} C_2(\text{so}(4, 2)) = & -\frac{3}{4} \left\{ \tilde{\eta}_4^2 \tilde{\xi}_4^2 + \tilde{\eta}_4 \tilde{\xi}_4 - 2\tilde{\eta}_3\tilde{\eta}_4\tilde{\xi}_3\tilde{\xi}_4 - 2\tilde{\eta}_2\tilde{\eta}_4\tilde{\xi}_2\tilde{\xi}_4 \right. \\ & + \tilde{\eta}_2 \tilde{\xi}_2 + \tilde{\eta}_3^2 \tilde{\xi}_3^2 + 2\tilde{\eta}_2\tilde{\eta}_3\tilde{\xi}_2\tilde{\xi}_3 + 2\tilde{\eta}_1\tilde{\eta}_4\tilde{\xi}_1\tilde{\xi}_4 + 2\tilde{\eta}_1\tilde{\eta}_3\tilde{\xi}_1\tilde{\xi}_3 + \tilde{\eta}_1 \tilde{\xi}_1 \\ & \left. + \tilde{\eta}_2^2 \tilde{\xi}_2^2 + \tilde{\eta}_1^2 \tilde{\xi}_1^2 + \tilde{\eta}_3 \tilde{\xi}_3 - 2\tilde{\eta}_1\tilde{\eta}_2\tilde{\xi}_1\tilde{\xi}_2 - 4 \right\}. \end{aligned} \quad (42.39)$$

From the comparison of expression (42.33) and (42.36) we obtain

$$C_2(\text{so}(4, 2)) = -\frac{3}{4} C_2(\text{u}(2, 2)) + \frac{3}{2}. \quad (42.40)$$

Thus the eigenvalue of $C_2(\text{so}(4, 2))$

$$g_2(\text{so}(4, 2)) = 3 \quad (42.41)$$

for the irreducible representation which is realized in the space of the bound states of the three-dimensional Coulomb problem. It belongs to the positive discrete series of the unitary irreducible representations of the $\text{so}(4, 2)$ algebra. It is unambiguously characterized by the eigenvalue (42.41) [7].

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Chapter IX

The Five-Dimensional Oscillator and Nuclear Collective Motions

After the discovery of the neutron by Chadwick [1] in 1932, one arrived at the concept that the nucleus of an atom was formed by a system of Z protons and $A-Z$ neutrons, where Z and A are respectively the atomic (*i.e.*, charge) and mass numbers of the nucleus in question.

From the beginning one tried to analyze the nucleus as a many-body system with a corresponding Schroedinger equation where, besides the kinetic energy, there was a short range potential between the nucleons. After many decades of effort [2], this *ab initio* approach failed as it turned out that the nucleons themselves were complex systems of (in our present view) quarks and gluons.

What was successful though was the introduction of simple models with the help of which many of the nuclear features were understood. One of them was the nuclear shell model [3] some of whose aspects were discussed in Chapter V within the framework of the Hartree–Fock approximation.

An even earlier model was the one of a liquid drop proposed by Niels Bohr [4] in 1936 which was so successful in the understanding of nuclear fission [5]. We shall consider this model, when limited just to small quadrupole vibrations, to derive for the Hamiltonian the five-dimensional oscillator, that was basic to the study of collective motions in nuclei initiated by Bohr and Mottelson [6]. This Hamiltonian will first be given in a frame of reference fixed in space and then in one fixed in the body, and it

will be for the latter that explicit eigenfunction will be obtained with the help of the $U(5) \supset O(5) \supset O(3)$ chain of groups.

We shall then consider the generalized operators of kinetic and potential energies in the quadrupole liquid drop model proposed by Greiner *et al.* [7], and discuss their matrix elements with respect to the eigenfunctions mentioned in the previous paragraph.

Finally the whole procedure will be applied to the analysis of the spectra of ^{238}U as well as some remarks on other nuclei.

43 The Quadrupole Liquid Drop Model and Its Classical Hamiltonian for Small Deformations

If the motion of the liquid drop is restricted to the quadrupole type the surface of the liquid drop is described by the equation

$$R = R_0 [1 + \sum_{m=-2}^2 \alpha^m Y_{2m}(\theta, \varphi)], \quad (43.1)$$

where R_0 is the spherical radius in the absence of deformation, $Y_{2m}(\theta, \varphi)$ is the quadrupole spherical harmonic and α^m , $m = 2, 1, 0, -1, -2$, the contravariant form of the coordinates describing the collective motion.

Note that as $Y_{2m}(\theta, \varphi)$ is a Racah tensor of second order the α^m must have the same characteristic and the relation between its contravariant and covariant form is

$$\alpha^m = (-1)^m \alpha_{-m} = \alpha_m^*. \quad (43.2)$$

The fluid inside the drop will be assumed irrotational and of constant density so the velocity \mathbf{v} of a volume element can be described by a potential ϕ as

$$\mathbf{v} = \nabla \phi, \quad (43.3)$$

and the continuity equation reduces to

$$\nabla \cdot \mathbf{v} = \nabla^2 \phi = 0. \quad (43.4)$$

As we are looking for a solution of (43.4) in the region inside the surface that includes the origin, the most general ϕ is a linear combination of the solid spherical harmonics $(r/R_0)^\ell Y_{\ell m}(\theta, \varphi)$. Because the surface has only quadrupole deformations we can restrict our ϕ to the form

$$\phi = \sum_{m=-2}^2 A^m (r/R_0)^2 Y_{2m}(\theta, \varphi). \quad (43.5)$$

As the radial velocity at the surface is

$$[(\mathbf{r}/r) \cdot \mathbf{v}]_{r=R_0} = [(\mathbf{r}/r) \cdot \nabla \phi]_{r=R_0} = (\partial \phi / \partial r)_{r=R_0}, \quad (43.6)$$

and it must be equal to $(\partial R / \partial t)$ we immediately obtain

$$R_0 \dot{\alpha}_m = (2/R_0) A^m, \quad (43.7)$$

where the dot here indicates derivative with respect to time.

Denoting by ρ the density of the liquid and by $d\tau$ the volume element the kinetic energy of the drop is given by

$$\begin{aligned} T &= (1/2)\rho \int \nabla \phi^* \cdot \nabla \phi d\tau \\ &= (R_0^2/2)\rho \int_0^\pi \int_0^{2\pi} (\mathbf{r}/r) \cdot (\phi^* \nabla \phi) \sin \theta d\theta d\varphi, \end{aligned} \quad (43.8)$$

where we made use of the fact that $\nabla \phi^* \cdot \nabla \phi = \nabla \cdot (\phi^* \nabla \phi)$ because $\nabla^2 \phi = 0$, as well as of Gauss theorem. From the relation $(\mathbf{r}/r) \cdot \nabla \phi = (\partial \phi / \partial r)$, and using (43.5) as well as (43.2) and the orthonormality of spherical harmonics, we obtain

$$T = R_0 \rho \sum_{m=-2}^2 A_m A^m = \frac{1}{2} B_2 \sum_{m=-2}^2 \dot{\alpha}_m \dot{\alpha}^m, \quad (43.9)$$

where the right hand side comes from using (43.7) while

$$B_2 = (1/2)R_0^5 \rho. \quad (43.10)$$

We turn now our attention to the potential energy, which is related to the change of shape of the nucleus. It consists of two terms:

$$V = V_s + V_c, \quad (43.11)$$

where V_s, V_c describe respectively the contribution to the potential of the surface tension and of the Coulomb repulsion of the protons.

As in all problems of small vibrations the potential energy should be a quadratic function of the deformation parameters and, besides, it should be invariant under rotations so it can only be proportional to $\sum_{m=-2}^2 \alpha^m \alpha_m$. A straightforward analysis [8] for the two terms V_s, V_c shows that the potential energy can be written as

$$V = \frac{1}{2}C_2 \sum_{m=-2}^2 \alpha_m \alpha^m, \quad (43.12)$$

where

$$C_2 = [4R_0^2\sigma - (3e^2Z^2/10\pi R_0)], \quad (43.13)$$

and the first term in the round bracket is due to the surface tension denoted by σ and the second to the change in the repulsive energy of the deformed liquid drop of charge Z , as shown in pp. 851–853 of reference [8].

The Lagrangian of the problem is $L = T - V$ and so the momentum is defined in the standard way by

$$\pi_m = \frac{\partial L}{\partial \dot{\alpha}^m} = B_2 \dot{\alpha}_m, \quad (43.14)$$

where the right hand side term comes from the expression (43.9) for the kinetic energy.

The Hamiltonian is in turn given by

$$H = \sum_{m=-2}^2 \pi_m \dot{\alpha}^m - L, \quad (43.15)$$

and so employing the relation (43.14) to express it in terms π_m, α_m alone, and using units in which

$$\hbar = B_2 = C_2 = 1, \quad (43.16)$$

we have that

$$H = \frac{1}{2} \sum_{m=-2}^2 (\pi_m \pi^m + \alpha_m \alpha^m) \quad (43.17)$$

both in the classical case where $\pi_m = \dot{\alpha}_m$ and in the quantum one in which

$$\pi_m = \frac{1}{i} \frac{\partial}{\partial \alpha^m}. \quad (43.18)$$

We are thus dealing with a five-dimensional oscillator, and if we introduce the creation and annihilation operators with the usual definition,

$$\eta_m = (1/\sqrt{2})(\alpha_m - i\pi_m), \quad \xi^m = (1/\sqrt{2})(\alpha^m + i\pi^m), \quad (43.19)$$

the quantum operator can also be written as

$$\hat{H} = \frac{1}{2} \sum_{m=-2}^2 (\eta_m \xi^m + \xi^m \eta_m) = \sum_{m=-2}^2 (\eta_m \xi^m) + (5/2), \quad (43.20)$$

as furthermore we have the commutation relation

$$[\xi^m, \eta_{m'}] = \delta_{m'}^m. \quad (43.21)$$

From the discussion in Chapter VII it is immediately clear that the symmetry Lie algebra of the Hamiltonian H is $u(5)$ and its dynamical group $Sp(10, R)$.

We shall make use of these properties when deriving later on the BIR of the $u(5)$ Lie algebra within a chain of appropriate subalgebras.

Finally as a last point we wish to rewrite Eq. (43.1) for the surface in cartesian form [8], i.e.,

$$R = R_0 \left(1 + \alpha_{xx} \frac{x^2}{r^2} + \alpha_{yy} \frac{y^2}{r^2} + \alpha_{zz} \frac{z^2}{r^2} + 2\alpha_{xy} \frac{xy}{r^2} + 2\alpha_{xz} \frac{xz}{r^2} + 2\alpha_{yz} \frac{yz}{r^2} \right), \quad (43.22)$$

where the relation between the cartesian α operators and the spherical ones $\alpha_m, m = 2, 1, 0, -1, -2$ are given in p. 39 of reference [8] as

$$\alpha_{\pm 2} = \left(\frac{8\pi}{15} \right)^{\frac{1}{2}} \frac{1}{2} (\alpha_{xx} - \alpha_{yy} \pm 2i\alpha_{xy}), \quad (43.23a)$$

$$\alpha_{\pm 1} = \mp \left(\frac{8\pi}{15} \right)^{\frac{1}{2}} (\alpha_{xz} \pm i\alpha_{yz}), \quad (43.23b)$$

$$\alpha_0 = \left(\frac{8\pi}{15} \right)^{\frac{1}{2}} \frac{1}{\sqrt{6}} \left[3\alpha_{zz} - (\alpha_{xx} + \alpha_{yy} + \alpha_{zz}) \right]. \quad (43.23c)$$

For fixed R, r and α 's Eq. (43.22) represents an ellipsoid with arbitrary orientation in the frame of reference fixed in space. It is convenient to pass from (x, y, z) to another frame of reference (x', y', z') in which the axis are parallel to the principal ones of the ellipsoid, so that the equation of the surface takes the form

$$R = R_0 \left(1 + \alpha'_{xx} \frac{x'^2}{r^2} + \alpha'_{yy} \frac{y'^2}{r^2} + \alpha'_{zz} \frac{z'^2}{r^2} \right). \quad (43.24)$$

In the α' 's system one has $\alpha'_{xy} = \alpha'_{xz} = \alpha'_{yz} = 0$, and if we denote the spherical components of α' as $a_m, m = 2, 1, 0, -1, -2$ we see from relations similar to (43.23) that

$$a_1 = a_{-1} = 0, \quad (43.25a)$$

$$a_2 = a_{-2}. \quad (43.25b)$$

Thus we are left only with two terms a_2, a_0 and following Bohr and Mottelson [6] we shall call them

$$a_0 = \beta \cos \gamma, \quad a_2 = \frac{1}{\sqrt{2}} \beta \sin \gamma. \quad (43.26)$$

The a_m can be obtained from the α_m by a rotation of Euler angles that we denote by $\vartheta_1, \vartheta_2, \vartheta_3$ and being Racah tensors of order 2, we have

$$a_{m'} = \sum_{m=-2}^2 \alpha_m D_{mm'}^2(\vartheta_1 \vartheta_2 \vartheta_3), \quad (43.27)$$

where $D_{mm'}^2(\vartheta_1 \vartheta_2 \vartheta_3)$ are the Wigner irreps for the rotation group as given in p. 52 of Rose's book [9].

We shall invert the relation (43.26) in the next section, to discuss the classical and quantum Hamiltonian of the five-dimensional harmonic oscillator in the frame of reference fixed in the body.

44 The Classical and Quantum Hamiltonians for Quadrupole Deformations in the Frame of Reference Fixed in the Body

From the unitarity properties of the D functions we have that [9]

$$\alpha_m = \sum_{m=-2}^2 D_{mm'}^{2*}(\vartheta_i) a_{m'}; \quad i = 1, 2, 3; \quad m = 2, 1, 0, -1, -2, \quad (44.1)$$

and thus the potential energy term in the Hamiltonian (43.17) becomes

$$\sum_{m=-2}^2 \alpha_m \alpha^m = \sum_{m=-2}^2 a_m a^m = \sum_{m=-2}^2 (-1)^m a_m a_{-m} = \beta^2, \quad (44.2)$$

where we made use of (43.26).

For the kinetic energy we start with the classical expression

$$\sum_{m=-2}^2 \pi_m \pi^m = \sum_{m=-2}^2 \dot{\alpha}_m \dot{\alpha}^m, \quad (44.3)$$

and thus our first objective will be to calculate

$$\begin{aligned} \dot{\alpha}_m &= \frac{\partial}{\partial t} \left[\sum_{m'=-2}^2 D_{mm'}^{2*}(\vartheta_i) a_{m'} \right] \\ &= \sum_{m'=-2}^2 \sum_{i=1}^3 \left(\frac{\partial D_{mm'}^{2*}}{\partial \vartheta_i} \dot{\vartheta}_i \right) a_{m'} + \sum_{m'=-2}^2 D_{mm'}^{2*}(\vartheta_i) \dot{a}_{m'}, \end{aligned} \quad (44.4)$$

with the dot indicating derivative with respect to time and where from (43.26), we see that

$$\dot{a}_2 = \dot{a}_{-2} = (1/\sqrt{2})(\dot{\beta} \sin \gamma + \beta \dot{\gamma} \cos \gamma), \quad (44.5a)$$

$$\dot{a}_1 = \dot{a}_{-1} = 0, \quad (44.5b)$$

$$\dot{a}_0 = \dot{\beta} \cos \gamma - \beta \dot{\gamma} \sin \gamma. \quad (44.5c)$$

To obtain then $\dot{\alpha}_m$ we need also to consider the derivatives

$$\frac{\partial D_{mm'}^{2*}(\vartheta_1 \vartheta_2 \vartheta_3)}{\partial \vartheta_i}, \quad (44.6)$$

which can be obtained from the explicit form of the $D_{mm'}^{2*}(\vartheta_i)$ functions in p. 52 of Rose's book [9].

It is more convenient to attack directly the problem of the classical kinetic energy, by using results derived by Eisenberg and Greiner [8]. For this purpose we introduce the coordinates q_ℓ , $\ell = 1, 2, 3, 4, 5$, where

$$q_i = \vartheta_i, \quad i = 1, 2, 3, \quad q_4 = \beta, \quad q_5 = \gamma, \quad (44.7)$$

and the kinetic energy becomes

$$T = (1/2) \sum_{m=-2}^2 (-1)^m \dot{\alpha}_m \dot{\alpha}_{-m} = (1/2) \sum_{\ell, \nu} g_{\ell \nu}(q) \dot{q}_\ell \dot{q}_\nu, \quad (44.8)$$

where the $g_{\ell \nu}(q)$, $\nu, \ell = 1, 2 \dots 5$, are given in p. 160 of reference [8] as

$$g_{11} = \Im_1 S_2^2 C_3^2 + \Im_2 S_2^2 S_3^2 + \Im_3 C_2^2,$$

$$g_{12} = g_{21} = -\Im_1 S_2 C_3 S_3 + \Im_2 S_2 S_3 C_3,$$

$$g_{22} = \Im_1 S_3^2 + \Im_2 C_3^2, \quad g_{23} = g_{32} = 0,$$

$$g_{13} = g_{31} = \Im_3 C_2, \quad g_{33} = \Im_3,$$

$$g_{44} = 1, \quad g_{55} = \beta^2,$$

$$g_{i4} = g_{4i} = 0, \quad g_{i5} = g_{5i} = 0, \quad i = 1, 2, 3, \quad g_{45} = g_{54} = 0, \quad (44.9)$$

with

$$C_i \equiv \cos \vartheta_i, S_i = \sin \vartheta_i, i = 1, 2, 3, \quad (44.10)$$

and \mathfrak{I}_i are the moments of inertia around the three axis of the body shown in p. 132 of reference [8] as

$$\mathfrak{I}_i = 4\beta^2 \sin^2(\gamma - \frac{2}{3}\pi i) \equiv \beta^2 I_i(\gamma). \quad (44.11)$$

The determinant of the 5×5 -dimensional matrix $g_{\ell\nu}$ can be written as

$$g \equiv \det \|g_{\ell\nu}\| = \beta^2 \det \|g_{ij}\|, \quad (44.12)$$

where g_{ij} , $i, j = 1, 2, 3$, are the components of the three-dimensional submatrix, so the determinant can be easily evaluated to give

$$g = \beta^2 \sin^2 \vartheta_2 \quad \mathfrak{I}_1 \mathfrak{I}_2 \mathfrak{I}_3 = 4\beta^8 \sin^2 \vartheta_2 \sin^2 3\gamma, \quad (44.13)$$

and so the volume element becomes

$$d\tau = 2\beta^4 \sin \vartheta_2 \sin 3\gamma d\vartheta_1 d\vartheta_2 d\vartheta_3 d\gamma d\beta. \quad (44.14)$$

The reciprocal of the matrix $\|g_{\ell\nu}\|$ whose components will be denoted as $(g^{-1})_{\ell\nu}$ are easy to evaluate as essentially they imply finding the reciprocal of the (3×3) matrix $\|g_{ij}\|$ through the use of the cofactors of its elements divided by its determinant, and the explicit values of $(g^{-1})_{\ell\nu}$ are also given in the page mentioned of reference [8].

If we want now the expression of the quantum mechanical kinetic energy operator \hat{T} , we can obtain it through the expression of Laplacian in curvilinear coordinates which is

$$\hat{T} = -\frac{1}{2} \sum_{\ell,\nu} \frac{1}{\sqrt{g}} \frac{\partial}{\partial q_\ell} \sqrt{g} (g^{-1})_{\ell\nu} \frac{\partial}{\partial q_\nu}, \quad (44.15)$$

and so finally the operator of the Hamiltonian associated with the five-dimensional oscillator becomes

$$\hat{H} = -\frac{1}{2} \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} + \frac{\mathcal{L}^2}{2\beta^2} + \frac{1}{2} \beta^2, \quad (44.16)$$

where, in turn [8],

$$\mathcal{L}^2 = -\frac{1}{\sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} + \sum_{i=1}^3 \frac{\hat{L}_i'^2}{I_i(\gamma)}, \quad (44.17)$$

where the $I_i(\gamma)$ are given by (44.11) while the \hat{L}_i' are the components of the angular momentum in the frame of reference fixed in the body which,

in terms of Euler angles, have the form given in p. 120 of reference [8], *i.e.*,

$$\hat{L}_1' = -i \left\{ -\frac{\cos \vartheta_3}{\sin \vartheta_2} \frac{\partial}{\partial \vartheta_1} + \sin \vartheta_3 \frac{\partial}{\partial \vartheta_2} + \cot \vartheta_2 \cos \vartheta_3 \frac{\partial}{\partial \vartheta_3} \right\} \quad (44.18a)$$

$$\hat{L}_2' = -i \left\{ \frac{\sin \vartheta_3}{\sin \vartheta_2} \frac{\partial}{\partial \vartheta_1} + \cos \vartheta_3 \frac{\partial}{\partial \vartheta_2} - \cot \vartheta_2 \sin \vartheta_3 \frac{\partial}{\partial \vartheta_3} \right\} \quad (44.18b)$$

$$\hat{L}_3' = -i \left\{ \frac{\partial}{\partial \vartheta_3} \right\}. \quad (44.18c)$$

We shall compare the Hamiltonian (44.16) for the five-dimensional oscillator with one of the three-dimensional oscillators:

$$\hat{\mathcal{H}} = -\frac{1}{2r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\hat{L}^2}{2r^2} + \frac{1}{2} r^2. \quad (44.19)$$

We know that this Hamiltonian is related to the first order Casimir operator of the U(3) group, *i.e.*,

$$\hat{\mathcal{H}} = \hat{\mathcal{N}} + (3/2), \quad (44.20a)$$

$$\hat{\mathcal{N}} = \boldsymbol{\eta} \cdot \boldsymbol{\xi}, \quad (44.20b)$$

while L^2 is the Casimir operator of the orthogonal subgroup O(3). On the other hand, from (43.20) we see that \hat{H} is related to the first order Casimir operator of U(5) so we expect \mathcal{L}^2 to be the Casimir operator of the O(5) group, as will be shown later to be the case.

Furthermore the Hamiltonian (44.20), as it is a contraction of a covariant and contravariant Racah tensors of rank 1, is a scalar and thus it remains invariant under the orthogonal group of rotations O(3) in space. The generators of this group are the components of angular momentum in the frame of reference fixed in space which, in terms of Euler angles, are given by the operators L_i , $i = 1, 2, 3$ given in p. 122 of reference [8], *i.e.*,

$$\hat{L}_1 = -i \left\{ -\cos \vartheta_1 \cot \vartheta_2 \frac{\partial}{\partial \vartheta_1} - \sin \vartheta_1 \frac{\partial}{\partial \vartheta_2} + \frac{\cos \vartheta_1}{\sin \vartheta_2} \frac{\partial}{\partial \vartheta_3} \right\} \quad (44.21a)$$

$$\hat{L}_2 = -i \left\{ -\sin \vartheta_1 \cot \vartheta_2 \frac{\partial}{\partial \vartheta_1} + \cos \vartheta_1 \frac{\partial}{\partial \vartheta_2} + \frac{\sin \vartheta_1}{\sin \vartheta_2} \frac{\partial}{\partial \vartheta_3} \right\} \quad (44.21b)$$

$$\hat{L}_3 = -i \left\{ \frac{\partial}{\partial \vartheta_3} \right\}. \quad (44.21c)$$

It is straightforward to verify that the commutation relations for the components \hat{L}_i of the angular momentum fixed in space are

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_k, \quad (44.22)$$

while those of L'_i fixed in the body are

$$[\hat{L}'_i, \hat{L}'_j] = -i\epsilon_{ijk}\hat{L}'_k, \quad (44.23)$$

and \hat{L}_i and \hat{L}'_i commute, i.e., $[\hat{L}_i, \hat{L}'_j] = 0$.

Finally the Casimir operator of $O(3)$ is expressed in the same way in both frames of reference and, as seen also in p. 122 of [8], is

$$\begin{aligned} \hat{L}^2 &\equiv \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2 = \hat{L}'_1^2 + \hat{L}'_2^2 + \hat{L}'_3^2 \\ &= \left\{ -\frac{\partial^2}{\partial \vartheta_2^2} - \cot \vartheta_2 \frac{\partial}{\partial \vartheta_2} - \frac{1}{\sin^2 \vartheta_2} \left(\frac{\partial^2}{\partial \vartheta_1^2} + \frac{\partial^2}{\partial \vartheta_3^2} \right) \right. \\ &\quad \left. + \frac{2 \cos \vartheta_2}{\sin^2 \vartheta_2} \frac{\partial^2}{\partial \vartheta_1 \partial \vartheta_3} \right\}. \end{aligned} \quad (44.24)$$

The states function of Euler angles that are basis for irreducible representations of the $O(3)$ group could be characterized by the eigenvalues $L(L+1), M, K$ of the commuting operators $\hat{L}^2, \hat{L}_3, \hat{L}'_3$ and they will be denoted by

$$D_{MK}^{L*}(\vartheta_1 \vartheta_2 \vartheta_3) = e^{iM\vartheta_1} d_{MK}^L(\vartheta_2) e^{iK\vartheta_3}, \quad (44.25)$$

with d_{MK}^L given in terms of ϑ_2 (called β in there) in Eq. (4.13) p. 52 of Rose's book [9].

In the same way that the eigenvalue of the Casimir operator \hat{L}^2 of $O(3)$ can be written as $L(L+1)$ where L is an nonnegative integer, the Casimir operator \mathcal{L}^2 of $O(5)$ has an eigenvalue of the form $\kappa(\kappa+3)$ where again κ is a nonnegative integer. This point will be proved in the next section, but here it indicates that in Eq. (44.16) we can replace \mathcal{L}^2 by $\kappa(\kappa+3)$ and we have an ordinary differential equation in β alone which allows to determine the part depending on this variable in the eigenfunction of the Hamiltonian (44.16).

The problem then reduces to finding eigenfunction χ of the operator

$$\mathcal{L}^2 \chi = \kappa(\kappa+3)\chi, \quad (44.26)$$

where $\chi = \chi(\gamma, \vartheta_1, \vartheta_2, \vartheta_3, \gamma)$. As \mathcal{L}^2 clearly commutes with L^2, L_3 we can develop χ in terms of the complete set of functions $D_{MK}^{L*}(\vartheta_i)$ with L, M fixed but K taking the allowed integer values $-L \leq K \leq L$.

We can thus reduce (44.26) to set off coupled ordinary differential equations in the variable γ , and so it is clear that the eigenstate of the Hamiltonian (44.16) associated with the chain of groups

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$$\begin{matrix} U(5) & \supset & O(5) & \supset & O(3) & \supset & O(2) \\ \nu & & \kappa & & L & & M \end{matrix} \quad (44.27)$$

can be written in the form of the ket [8]

$$|\nu \kappa \ell LM\rangle = F_j^\kappa(\beta) \sum_K \phi_K^{\kappa \ell L}(\gamma) \left[D_{MK}^{L*}(\vartheta_i) + (-1)^L D_{M-K}^{L*}(\vartheta_i) \right], \quad (44.28)$$

where ν is the total number of quanta given by

$$\nu = 2j + \kappa; \quad j = 0, 1, 2, \dots \quad \kappa = 0, 1, 2, \dots, \quad (44.29)$$

and so the eigenvalue of \hat{H} of (44.16) is $\nu + (5/2)$. The indices ν, κ, L, M indicate respectively the irreps of the groups $U(5)$, $O(5)$, $O(3)$, $O(2)$, and, as irreps L of $O(3)$ can appear more than once in an irrep κ of $O(5)$ we introduced an extra index ℓ whose characteristics will be discussed in the next section.

From symmetry considerations associated with the choice of principal axis, as discussed in page 184 of reference [8], we cannot develop the function χ exclusively in terms of $D_{MK}^{L*}(\vartheta_i)$, but must use the combination that appears in the square bracket in (44.28), with the further restriction that in there

$$K = 0, 2, \dots, L \text{ for } L \text{ even,} \quad (44.30a)$$

$$K = 0, 2, \dots, L-1 \text{ for } L \text{ odd.} \quad (44.30b)$$

Clearly then the eigenkets of the five-dimensional harmonic oscillator are fully determined if we can obtain $\phi_K^{\kappa \ell L}(\gamma)$, as $D_{MK}^{L*}(\vartheta_i)$ was given in (44.25) and the ordinary differential equation in β given by \hat{H} of (44.16), when \mathcal{L}^2 is replaced by $\kappa(\kappa+3)$, has an orthonormalized set of solutions of the form

$$F_j^\kappa(\beta) = \left[\frac{2(j!)}{\Gamma(j+\kappa+\frac{5}{2})} \right]^{\frac{1}{2}} \beta^\kappa L_j^{\kappa+\frac{3}{2}}(\beta^2) \exp(-\beta^2/2), \quad (44.31)$$

with $L_j^{\kappa+3/2}$ being a Laguerre polynomial.

As mentioned above the functions that in (44.28) we denote by $\phi_K^{\kappa \ell L}(\gamma)$ satisfy a set of coupled ordinary differential equations. Bes [10] gave a recurrence procedure for deriving $\phi_K^{\kappa \ell L}(\gamma)$ for $L = 0, 2, 3, 4, 5, 6$, but we propose to show that, using group theoretical arguments, $\phi_K^{\kappa \ell L}(\gamma)$ can be determined in general.

For our latter program it is necessary to discuss two particular cases of equation (44.26) corresponding to $L = 0$ and $L = 3$.

If $L = 0, K = 0$ the application of the \hat{L}'_i operators to constant D_{00}^0 gives 0 so we are led to the equation

$$-\frac{1}{\sin 3\gamma} \frac{d}{d\gamma} \sin 3\gamma \frac{d}{d\gamma} \phi_0^{\kappa L 0}(\gamma) = \kappa(\kappa + 3)\phi_0^{\kappa L 0}(\gamma). \quad (44.32)$$

A regular solution is possible only if κ is a multiple of 3 and we define ℓ in this case by requiring

$$\kappa = 3\ell, \quad (44.33)$$

so that $\phi_0^{3\ell, \ell, 0}$ is proportional to the Legendre polynomial $P_\ell(\cos 3\gamma)$.

It is convenient now to limit our discussion to states $|\nu \kappa \ell LM\rangle$ of (44.28) in which $\nu = \kappa$ and $M = L$ and call them

$$|\kappa \ell L\rangle = |\nu = \kappa, \kappa, \ell, L, M = L\rangle, \quad (44.34)$$

as $|\nu \kappa \ell LM\rangle$ can be obtained from them by introducing the Laguerre polynomial $L_j^{\kappa+\frac{3}{2}}(\beta^2)$ and applying the lowering operator $L_{-1} = L_1 - iL_z$.

For $L = 0$ we have then that

$$|3\ell, \ell, 0\rangle = A_\ell \beta^{3\ell} \exp(-\beta^2/2) P_\ell(\cos 3\gamma), \quad (44.35)$$

where A_ℓ is, so far, an arbitrary constant that we shall later select conveniently.

Turning now our attention to odd L we note that the square bracket in (44.28) vanishes identically if $L = 1$ because from (44.30) K can only take the value 0. We look then to $L = 3$ for which $K = 0, 2$, but again $K = 0$ vanishes, so we get only a single ordinary differential equation:

$$\left[-\frac{1}{\sin 3\gamma} \frac{d}{d\gamma} \sin 3\gamma \frac{d}{d\gamma} + \frac{9}{\sin^2 3\gamma} \right] \phi_2^{\kappa \ell 3}(\gamma) = \kappa(\kappa + 3)\phi_2^{\kappa \ell 3}(\gamma), \quad (44.36)$$

where we used the fact that [11]

$$(7/8\pi^2) \int D_{3\pm 2}^3(\vartheta_i) \hat{L}_k'^2 D_{3\pm 2}^{3*}(\vartheta_i) d\Omega = 4; \quad k = 1, 2, 3, \quad (44.37)$$

with $d\Omega = \sin \vartheta_2 d\vartheta_1 d\vartheta_2 d\vartheta_3$, and also that

$$\frac{1}{\sin^2 \gamma} + \frac{1}{\sin^2(\gamma - \frac{2\pi}{3})} + \frac{1}{\sin^2(\gamma - \frac{4\pi}{3})} = \frac{9}{\sin^2 3\gamma}. \quad (44.38)$$

As in the case of $L = 0$ a regular solution exists only if $\kappa \equiv 0, \text{mod } 3$ and, for later convenience, in the case $L = 3$ we write

$$\kappa = 3\ell + 3. \quad (44.39)$$

We have then that $\phi_2^{3\ell+3, \ell, 3}(\gamma)$ will be proportional to an associated Legendre polynomial $P_{\ell+1}^1(\cos 3\gamma)$, and the corresponding state (44.34) becomes

$$|3\ell + 3, \ell, 3\rangle = B_\ell \beta^{3\ell+3} \exp(-\beta^2/2) P_{\ell+1}^1(\cos 3\gamma) [D_{3,2}^{3*}(\vartheta_i) - D_{3,-2}^{3*}(\vartheta_i)], \quad (44.40)$$

where B_ℓ is again an arbitrary constant to be selected later.

We shall now proceed to derive in a systematic fashion the states $|\kappa \ell L\rangle$ for arbitrary L starting from $L = 0$ if L is even, or $L = 3$ if L is odd.

45 States of the Five-Dimensional Oscillator Characterized by the Irreducible Representations of the Chain of Groups $U(5) \supset O(3)$

We shall proceed to obtain the eigenstates of the Hamiltonian of Eq. (43.20) that have definite angular momentum L , but with highest projection, i.e., $M = L$.

We shall express these states as polynomials in the creation operators η_m , $m = 2, 1, 0, -1, -2$, of (43.19a), acting on the ground state

$$|0\rangle = \frac{1}{2}\pi^{-5/4} \exp(-\beta^2/2), \quad (45.1)$$

which was normalized with respect the volume element (44.14) with the following range in the variables

$$0 \leq \vartheta_1, \vartheta_3 \leq 2\pi, \quad 0 \leq \vartheta_2 \leq \pi, \quad (45.2)$$

$$0 \leq \gamma \leq \pi/3, \quad 0 \leq \beta \leq \infty. \quad (45.3)$$

Because of the commutation rules (43.21) the annihilation operator ξ^m can be interpreted as

$$\xi^m = \partial/\partial \eta_m, \quad (45.4)$$

with the relation between contravariant and covariant components being given again in (43.2).

The number operator has then the form

$$\hat{N} = \sum_{m=-2}^2 \eta_m \xi^m = \hat{H} - (5/2), \quad (45.5)$$

and the components of angular momentum are given, by a reasoning similar to (38.11d), in the form

$$\hat{L}_q = -\sqrt{30} \sum_{mm'} (-1)^{m'} \begin{pmatrix} 2 & 1 & 2 \\ m & q & -m' \end{pmatrix} \eta_{m'} \xi^m, \quad q = 1, 0, -1, \quad (45.6)$$

implying in particular that

$$\hat{L}_1 = - \sum_{m=-2}^2 \left[(1/2)(3+m)(2-m) \right]^{\frac{1}{2}} \eta_{m+1} \xi^m, \quad (45.7a)$$

$$\hat{L}_0 = \sum_{m=-2}^2 (m \eta_m \xi^m). \quad (45.7b)$$

Note that we use here the same letter \hat{L} as in Chapter VII, but in this and the following Chapter they refer to the *five-dimensional* oscillator, while in Chapter VII we consider the *three-dimensional* oscillator.

We are now in search of the polynomials $P(\eta_m)$ that satisfy the equations [11]

$$\hat{N}P = \nu P, \quad (45.8a)$$

$$\hat{L}_1 P = 0, \quad (45.8b)$$

$$\hat{L}_0 P = L P, \quad (45.8c)$$

where the ξ^m in the operators is interpreted in the differential from (45.4).

The first equation in (45.8) implies that P is a homogeneous polynomial in the η 's and thus we can write it as

$$P(\eta_m) = \eta_2^\nu P' \left(\frac{\eta_1}{\eta_2}, \frac{\eta_0}{\eta_2}, \frac{\eta_{-1}}{\eta_2}, \frac{\eta_{-2}}{\eta_2} \right), \quad (45.9)$$

where P' is an arbitrary polynomial in the variables indicated of degree not exceeding ν . To apply the second equation of (45.8) we shall introduce the following polynomial functions:

$$(2, 0) \equiv \sum_{m=-2}^2 (-1)^m \eta_m \eta_{-m}, \quad (45.10a)$$

$$(3, 3) \equiv 7\sqrt{10/3} \sum_{mm'} \sum_{m''m'''} \begin{pmatrix} 2 & 2 & 2 \\ m & m' & -m''' \end{pmatrix} \times \begin{pmatrix} 2 & 2 & 3 \\ m''' & m'' & -3 \end{pmatrix} \eta_m \eta_{m'} \eta_{m''}, \quad (45.10b)$$

$$(2, 2) \equiv \sqrt{35} \sum_{mm'} (-1)^{m'''} \begin{pmatrix} 2 & 2 & 2 \\ m & m' & -2 \end{pmatrix} \eta_m \eta_{m'}, \quad (45.10c)$$

where in the last term of (45.10c) we use a Racah tensor product notation [9] that will also be employed later.

The notation is (ν, L) indicating the number of quanta ν , and the maximum projection $M = L$ of the angular momentum L of the polynomials, which correspond to elementary permissible diagrams (epd) in $U(5) \supset O(3)$, are similar to those in (38.33) for the chain $U(3) \supset O(3)$.

From the explicit form of the $3j$ coefficients in (45.10) we obtain

$$\frac{(2, 0)}{\eta_2^2} = 2 \frac{\eta_{-2}}{\eta_2} - \frac{1}{2} \frac{\eta_{-1}}{\eta_2} \frac{\eta_1}{\eta_2} + \frac{\eta_0^2}{\eta_2^2}, \quad (45.11a)$$

$$\frac{(3, 3)}{\eta_2^3} = 2 \frac{\eta_{-1}}{\eta_2} - \sqrt{6} \frac{\eta_1}{\eta_2} \frac{\eta_0}{\eta_2} + \frac{\eta_1^3}{\eta_2^3}, \quad (45.11b)$$

$$\frac{(2, 2)}{\eta_2^2} = 2\sqrt{2} \frac{\eta_0}{\eta_2} - \sqrt{3} \frac{\eta_1^2}{\eta_2^2}, \quad (45.11c)$$

and therefore we could also write P as [11]

$$P(\eta_m) = \eta_2^\nu P'' \left(\frac{\eta_1}{\eta_2}, \frac{(2, 2)}{\eta_2^2}, \frac{(3, 3)}{\eta_2^3}, \frac{(2, 0)}{\eta_2^2} \right), \quad (45.12)$$

where P'' is again an arbitrary polynomial of the variables indicated.

We note now that from their definition,

$$\hat{L}_1 \eta_2 = \hat{L}_1 (2, 0) = \hat{L}_1 (3, 3) = \hat{L}_1 (2, 2) = 0, \quad (45.13a)$$

$$\hat{L}_1 \eta_1 = -\sqrt{2} \eta_2, \quad (45.13b)$$

and thus, as L_1 given by (45.7a) is a first-order differential operator in the η 's, we have

$$\hat{L}_1 P = -\sqrt{2} \eta_2^\nu \frac{\partial P''}{\partial (\eta_1/\eta_2)} = 0, \quad (45.14)$$

which implies that P'' is independent of (η_1/η_2) and therefore we can write

$$P = \sum_{n_1 n_2 n_3} \left\{ B_{n_1 n_2 n_3} (2, 0)^{n_1} (3, 3)^{n_2} (2, 2)^{n_3} \eta_2^{\nu - 2n_1 - 3n_2 - 2n_3} \right\}, \quad (45.15)$$

where, so far, the $B_{n_1 n_2 n_3}$ are arbitrary constants.

Considering Eq. (45.8c) we see from (45.7b) and (45.15) that it implies

$$3n_2 + 2n_3 + 2(\nu - 2n_1 - 3n_2 - 2n_3) = L, \quad (45.16)$$

from which we obtain

$$n_3 = \frac{1}{2}(2\nu - L - 3n_2) - 2n_1. \quad (45.17)$$

Thus the polynomial that satisfies Eqs. (45.8) has the form

$$P(\eta_m) = \sum_{n_1, n_2} \left\{ B'_{n_1 n_2} \eta_2^{L - \nu + 2n_1} (2, 0)^{n_1} \times (3, 3)^{n_2} (2, 2)^{(2\nu - L - 3n_2)/2 - 2n_1} \right\}. \quad (45.18)$$

We note from (45.18) that for P to be a polynomial, n_2 must be even (odd) if $2\nu - L$, and thus also L , is even (odd). At first sight the different polynomials seem to be given by taking $B'_{n_1 n_2} = 1$ for a particular n_1, n_2 and zero for the rest, with the restriction that all the exponents are nonnegative. We note though that η_2 contains n_1 but not n_2 in its exponent. Thus there is the possibility that

$$\sum_{n_2} B'_{n_1 n_2} (3, 3)^{n_2} (2, 2)^{(2\nu - L - 3n_2)/2 - 2n_1} \quad (45.19)$$

for some coefficients of $B'_{n_1 n_2}$ could be divisible by η_2 , and in this case the exponent of η_2 can take negative values. To avoid this problem we note that the polynomial characterized by the epd (3,0), *i.e.*,

$$(3, 0) \equiv \sqrt{35} \sum_{mm'm''} \binom{2}{m} \binom{2}{m'} \binom{2}{m''} \eta_m \eta_{m'} \eta_{m''} \quad (45.20)$$

is related with those of (45.10) by

$$-(3\sqrt{3}/4)(3, 3)^2 = \eta_2^3 (3, 0) - \frac{3}{2} (2, 2)(2, 0) \eta_2^2 + \frac{1}{4} (2, 2)^3. \quad (45.21)$$

Thus if L is even, then n_2 is also even, *i.e.*,

$$n_2 = 2\ell, \quad (45.22)$$

and we can express $(3, 3)^{2\ell}$ in terms of $(3, 0)^\ell$ and powers of the other epd's. Therefore for $2\nu - L$ even, we can also write (45.18) as

$$P(\eta_m) = \sum_{n_1 \ell} \left\{ B''_{\ell n_1} \eta_2^{L - \nu + 2n_1 + 3\ell} \times (2, 2)^{(2\nu - L)/2 - 3\ell - 2n_1} (3, 0)^\ell (2, 0)^{n_1} \right\}. \quad (45.23)$$

It seems at first sight that we have not avoided the problem of divisibility in (45.23) as we can write

$$2n_1 + 3\ell = \tau, \quad (45.24)$$

and expressing n_1 in terms of τ we have now to ask whether

$$\mathcal{P}(\eta_m) \equiv \sum_\ell B'''_{\ell \tau} (3, 0)^\ell (2, 0)^{(\tau - 3\ell)/2} \quad (45.25)$$

is divisible by η_2 for some value of the coefficients $B'''_{\ell \tau}$. The answer to this last question is immediate. The polynomial (45.25) corresponds to $L = 0$ as the two epd (3,0), (2,0) appearing in it have angular momentum zero. Thus if we can factorize it in the form

$$\mathcal{P}(\eta_m) = \eta_2^x \mathcal{R}(\eta_m), \quad (45.26)$$

where x is some positive integer, then

$$L_1 \mathcal{R} = 0, \quad L_0 \mathcal{R} = -2x \mathcal{R}. \quad (45.27)$$

This implies that \mathcal{R} is a polynomial in the η'_m 's corresponding to a negative angular momentum which is clearly impossible.

We have then from (45.23) that the different polynomials are given by [11]

$$P_{\nu \ell L n_1}(\eta_m) = \eta_2^{L - \nu + 2n_1 + 3\ell} (2, 2)^{(2\nu - L)/2 - 3\ell - 2n_1} (3, 0)^\ell (2, 0)^{n_1} \quad (45.28)$$

when L is even, and ℓ, n_1, L and ν are restricted by the fact that all exponents must be nonnegative.

A similar analysis for odd L , in which case n_2 is odd and can be written as

$$n_2 = 2\ell + 1, \quad (45.29)$$

leads to [11]

$$P_{\nu L n_1}(\eta_m) = (3, 3) \eta_2^{L-\nu+2n_1+3\ell} \times (2, 2)^{(2\nu-L-3)/2-3\ell-2n_1} (3, 0)^\ell (2, 0)^{n_1}, \quad (45.30)$$

where again ℓ , n_1 , L and ν are restricted by the fact that all exponents must be nonnegative.

The polynomials (45.28), besides being characterized by the IR ν of $U(5)$ and L of $O(3)$, have two other labels, the nonnegative integers ℓ, n_1 which indicate the powers of the operators associated with the epd $(2,0)$, $(3,0)$.

We have obtained the complete, though not necessarily orthonormal, set of states of definite number of quanta ν and maximum projection of angular momentum $M = L$. For arbitrary M we just have to apply $(\hat{L}_{-1})^{L-M}$ of (45.6) to the polynomials. The states (45.28) do not correspond though to a given seniority, (*i.e.*, definite eigenvalue of the Casimir operator of $O(5)$) and in the next section we indicate how we can introduce this label in the classification scheme.

46 States Associated with the Chain $U(5) \supset O(5) \supset O(3)$ in Terms of Traceless Boson Operators

The polynomials derived in the previous section are characterized by the total number of quanta ν , *i.e.*, the irrep of $U(5)$ as well as by the total angular momentum L , *i.e.*, the irrep of $O(3)$. Both of the groups mentioned are given in terms of unitary matrices of 5×5 dimensions, which is obvious for $U(5)$, but in the case of $O(3)$ it means that we take its complex matrix representation of order 2, *i.e.*,

$$\|D_{mk}^2(\vartheta_1 \vartheta_2 \vartheta_3)\|, \quad m, k = 2, 1, 0, -1, -2. \quad (46.1)$$

Clearly between the general five-dimensional matrix $U(5)$ and the representation (46.1) of $O(3)$, we can introduce an orthogonal matrix of 5×5 dimensions in complex form associated with the group $O(5)$.

If we turn to the Lie algebras, the generators of our chain will be given respectively by

$$C_m^m = \eta_m \xi^m = (-1)^m \eta_m \xi_{-m}, \quad m, m' = 2, 1, 0, -1, -2, \quad (46.2)$$

for $U(5)$, and by the antisymmetric part [12] of C_m^m in its covariant form, *i.e.*,

$$\mathcal{L}_{mm'} \equiv \frac{1}{\sqrt{2}} (C_{m,m'} - C_{m',m}) \quad (46.3)$$

46. STATES ASSOCIATED WITH CHAIN $U(5) \supset O(5) \supset O(3)$

when we are dealing with $O(5)$, and by the operator L_q , $q = 1, 0, -1$ of (45.6) when we consider the generators of $O(3)$.

The polynomials (45.28,30) of our previous section when applied to the ground state $|0\rangle$ of (45.1), are eigenstates of the Casimir operators \hat{N} and \hat{L}^2 of $U(5)$ and $O(3)$ respectively, with eigenvalues ν and $L(L+1)$ and now we wish to characterize them also as eigenstates of the Casimir operator \mathcal{L}^2 of $O(5)$ defined by [12]

$$\begin{aligned} \mathcal{L}^2 &= \sum_{m,m'=-2}^2 \mathcal{L}_{m,m'} \mathcal{L}^{m',m} \\ &= \hat{N}(\hat{N} + 3) \left(\sum_{m'=-2}^2 \eta_{m'} \eta^{m'} \right) - \left(\sum_{m=-2}^2 \xi_m \xi^m \right), \end{aligned} \quad (46.4)$$

where the right hand side follows from (46.3) if we use the definition $\hat{N} = \sum_m \eta_m \xi^m$.

We mentioned in (44.26) that the eigenvalues of \mathcal{L}^2 are $\kappa(\kappa+3)$ with κ being an integer that can take the values $\kappa = \nu, \nu-2, \dots, 1$ or 0, and thus to achieve the purpose of the previous paragraph we must require that our state satisfies the equation

$$\mathcal{L}^2 P(\eta_m) |0\rangle = \kappa(\kappa+3) P(\eta_m) |0\rangle, \quad (46.5)$$

with $P(\eta_m)$ being the general polynomial in the creation operators given by (45.23) whose coefficients B''_{ℓ,n_1} , would be partially determined by Eq. (46.5).

We proceed to discuss Eq. (46.5) by first noting that from (44.28) we can restrict ourselves to the value $\nu = \kappa$, as when this case is determined, and we write the wave function in terms of $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$, the general case $\nu = \kappa + 2j$, can be obtained by multiplying the state with $\nu = \kappa$ by an appropriately normalized Laguerre polynomial $L_j^{\kappa+\frac{3}{2}}(\beta^2)$ as shown in (44.31).

If $\nu = \kappa$ we see from (46.4) that Eq. (46.5) is satisfied if we require that

$$\sum_{m=-2}^2 (\xi_m \xi^m) P(\eta_m) |0\rangle = 0, \quad (46.6)$$

where $P(\eta_m)$ is a polynomial that satisfies the condition (45.8) but with ν replaced by κ , and besides is “harmonic”, *i.e.*, it obeys (46.6).

If we take the polynomials $P_{\nu L n_1}(\eta_m)$ of (45.28) with $\nu = \kappa$, we find that they do not satisfy the condition (46.6). There is however a method,

originated by Vilenkin [13] and further developed by Lohe [14], by means of which we can enforce the condition (46.6) in a relatively simple way.

Following these authors [13,14] we introduce “traceless boson operators” defined by

$$\hat{a}_m^+ \equiv \eta_m - (2,0)(2\hat{N} + 5)^{-1}\xi_m, \quad m = 2, 1, 0, -1, -2, \quad (46.7)$$

where \hat{N} is the number operator of Eq. (45.5) and $(2,0)$ is the second degree polynomial of angular momentum 0 of Eq. (45.10a), *i.e.*, the one associated with two paired quanta. Using the identities

$$(2\hat{N} + 5)^{-1}\eta_m = \eta_m(2\hat{N} + 7)^{-1}, \quad (46.8a)$$

$$(2\hat{N} + 5)^{-1}\xi_m = \xi_m(2\hat{N} + 3)^{-1}, \quad (46.8b)$$

which hold when we apply the operators to homogeneous polynomials in the η 's, we can easily show that

$$[\hat{a}_m^+, \hat{a}_{m'}^+] = 0, \quad (46.9)$$

and furthermore that

$$\sum_{m=-2}^2 \hat{a}_m^+ \hat{a}^{+m} = (4\hat{N}^2 - 1)^{-1}(2,0)^2 \sum_{m=-2}^2 \xi_m \xi^m. \quad (46.10)$$

We now turn our attention to the polynomial $P_{\kappa\ell L n_1}(\eta_m)$ of (45.28). If we replace the η_m by \hat{a}_m^+ in these polynomials and apply them to the ground state $|0\rangle$ we see from (46.10) that the corresponding states will vanish unless $n_1 = 0$. Assuming this last condition and taking $\nu = \kappa$, we have the states

$$|\kappa\ell L\rangle = P_{\kappa\ell L 0}(\hat{a}_m^+)|0\rangle. \quad (46.11)$$

These states are linear combinations of terms like

$$\eta_{m_1} \eta_{m_2} \dots \eta_{m_k} |0\rangle, \quad (46.12)$$

i.e., they are homogeneous of degree κ in η_m , and they continue to be characterized by the angular momentum L . Moreover, if we apply $\sum_m \hat{a}_m^+ \hat{a}^{+m}$ on the state $|\kappa\ell L\rangle$ we obtain from Eqs. (46.9) and (46.10)

$$\begin{aligned} & (4\hat{N}^2 - 1)^{-1}(2,0)^2 \sum_m \xi_m \xi^m |\kappa\ell L\rangle \\ &= [P_{\kappa\ell L 0}(\hat{a}_m^+)](4\hat{N}^2 - 1)^{-1}(2,0)^2 \sum_m \xi_m \xi^m |0\rangle = 0, \end{aligned} \quad (46.13)$$

and since $(4\hat{N}^2 - 1)^{-1}(2,0)^2$ does not vanish identically, it follows that the states $P_{\kappa\ell L 0}(\hat{a}_m^+)|0\rangle$ are harmonic, *i.e.*, they satisfy condition (44.6). Thus the states (46.11) correspond to the irrep $(\kappa 0)$ of O(5) and $[\kappa 0000]$ of U(5), as we require a partition involving two numbers to characterize the general irreps [12] of O(5) and five numbers [12] for the irreps of U(5).

The “harmonic” states $|\kappa\ell L\rangle$ could then be obtained from the polynomials (45.28) applied to the ground state $|0\rangle$ of (45.1) when $n_1 = 0$ and we make the replacements

$$\eta_2 \rightarrow \hat{a}_2^+ \equiv [1, 2], \quad (46.14a)$$

$$(\nu, L) \rightarrow [\nu, L], \quad (46.14b)$$

where $[\nu, L]$ is given by the same definition (45.10) of (ν, L) but with \hat{a}_m^+ replacing η_m .

The above formulation of the kets $|\kappa\ell L\rangle$, which involves only *creation* traceless operators \hat{a}_m^+ , is not very convenient to transform the polynomials in these kets to purely ones involving ordinary creation operators η_m , which later on, by using a theorem of Dragt [15], can allow us to convert the kets $|\kappa\ell L\rangle$ into explicit wave functions depending on $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$.

Thus we shall proceed to consider a formulation of the ket $|\kappa\ell L\rangle$ in a particle-hole traceless operator picture. For this purpose we first consider the kets $L = 0$ so that from the discussion proceeding (46.14) we get

$$|\kappa\ell 0\rangle = [1, 2]^{-\kappa+3\ell} [2, 2]^{\kappa-3\ell} [3, 0]^\ell |0\rangle, \quad (46.15)$$

which clearly implies that $\kappa = 3\ell$ as all the exponents must be nonnegative, and we have the “harmonic” state

$$[3\ell, \ell, 0] = [3, 0]^\ell |0\rangle, \quad (46.16)$$

which should be identical to (44.35) if the constant A_ℓ appearing there is appropriately selected.

Clearly if we apply a power of the annihilation operator ξ_2 to (46.16) it remains harmonic as it commutes with $\sum_m \xi^m \xi_m$ and it will have definite angular momentum, with maximum projection $M = L$ as $[\hat{L}_1, \xi_2] = [\hat{L}_1, \xi^{-2}] = 0$ with \hat{L}_1 given by (45.7a).

After introducing a power of ξ_2 , we could apply a power of \hat{a}_2^+ , as from (46.9) and (46.10) we see that again the state remains harmonic and furthermore of definite angular momentum as $[L_1, \hat{a}_2^+] = 0$.

Thus in a *particle-hole* traceless boson formulation our states could be written as

$$|\kappa, \ell, L\rangle = (\hat{a}_2^+)^{\sigma} \xi_2^\tau [3, 0]^{\ell+\tau} |0\rangle, \quad (46.17)$$

where we have the following relations between the exponents:

$$\sigma + \tau = (L/2), \quad \text{which implies that } L \text{ is even,} \quad (46.18a)$$

$$\sigma + 2\tau + 3\ell = \kappa, \quad (46.18b)$$

$$\sigma, \tau, \ell, \text{ nonnegative integers.} \quad (46.18c)$$

When, for a fixed κ , we consider all the possible nonnegative integer values that σ, τ, ℓ can take, and for each possible L we include also its degeneracy $(2L+1)$ we showed, from the discussion after Eq. (2.9) of ref. [16] and that given in Appendix A of reference [11], that the number S of states of the type $|\kappa\ell LM\rangle$ with $M = L, L-1, \dots, -L$, is given by

$$S = (1/6)(\kappa+1)(\kappa+2)(2\kappa+3), \quad (46.19)$$

which is exactly the dimension of the irrep $(\kappa 0)$ of $O(5)$. Thus we have the full set of "harmonic" states we are looking for, at least for the case when L is even. In the following sections we shall proceed to write these states as polynomials in the ordinary creation operator η_m acting on the ground state and then as polynomials in the α_m introduced at the beginning of the Chapter, to end finally with states functions of $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$ of the form (44.28), i.e., we shall determine explicitly the function $\phi_K^{\kappa\ell L}(\gamma)$ appearing there.

The discussion of the full problem when L is odd, will be given in section 51.

47 The Expression of the States $|\kappa\ell L\rangle$ When L Is Even, in Terms of Polynomials in the EPD's of Creation Operators η_m and of the α_m

The state $|\kappa\ell L\rangle$ of (46.17) is given as a product of elementary permissible diagrams (epd) in traceless boson creation and annihilation operators. In this section we wish to express them as a polynomial in the epd of the ordinary creation operator η_m acting on the ground state. To achieve this purpose we start from the state with $L=0$ which from (45.28a) must have the form

$$|3\ell, \ell, 0\rangle = [3, 0]^\ell |0\rangle = \sum_r B_r^\ell (2, 0)^{3r} (3, 0)^{\ell-2r} |0\rangle. \quad (47.1)$$

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The coefficients B_r^ℓ where obtained by Cowan and Sharp [17] by applying $\sum_m (-1)^m \xi_m \xi_{-m}$ to (47.1), which must then vanish, and getting a recursion relation for the B_r^ℓ which they solved. Another procedure consists in remembering that the state (47.1) has the form (44.35), i.e.,

$$\begin{aligned} |3\ell, \ell, 0\rangle &= \beta^{3\ell} P_\ell(x) e^{-\beta^2/2} \\ &= \beta^{3\ell} \sum_r \frac{(-1)^r (2\ell - 2r - 1)!!}{2^r r!(\ell - 2r)!} x^{\ell-2r} e^{-\beta^2/2} \\ &= \frac{(-1)^\ell}{2^{\ell/2}} \sum_r (-1)^r \frac{(2\ell - 2r - 1)!!}{r!(\ell - 2r)!} \\ &\quad \times \{2, 0\}^{3r} \{3, 0\}^{\ell-2r} e^{-\beta^2/2}, \end{aligned} \quad (47.2)$$

where we now denote by curly brackets $\{\nu, L\}$ the same expressions (ν, L) of (45.10) but with η_m replaced by α_m and thus, in particular, we have

$$\{2, 0\} = \sum_m \alpha^m \alpha_m = \beta^2, \quad (47.3a)$$

$$\begin{aligned} \{3, 0\} &= \sqrt{35} \sum_{mm'm''} \binom{2}{m} \binom{2}{m'} \binom{2}{m''} \alpha_m \alpha_{m'} \alpha_{m''} \\ &= -\sqrt{2}\beta^3 \cos 3\gamma = -\sqrt{2}\beta^3 x, \end{aligned} \quad (47.3b)$$

where from now on we shall use the shorthand notation

$$\cos 3\gamma = x. \quad (47.4)$$

Comparing now (47.1) and (47.2), where the polynomials satisfy the same equations, only that in the first case they are functions of the η_m and in the second of the α_m , we conclude that we can take

$$B_r^\ell = \frac{(-1)^r (2\ell - 2r - 1)!!}{r!(\ell - 2r)!}, \quad (47.5)$$

as the states $|\kappa\ell L\rangle$ are not normalized and thus have an arbitrary multiplicative constant.

We want now to extend the development (47.1) to states with arbitrary even L . We shall indicate how to extend all the results obtained so far to odd angular momentum in Section 51.

As the states $|\kappa\ell L\rangle$ can be written in the form

$$|\kappa\ell L\rangle = (\hat{a}_2^+)^\sigma \xi_2^\tau |3\ell + 3\tau, \ell + \tau, 0\rangle, \quad (47.6)$$

we see that the application of operator ξ_2 to (47.1) is simple as $\xi_2 = \partial/\partial\eta_{-2}$. On the other hand, from the form (46.7) of \hat{a}_m^+ we see that application of

powers \hat{a}_m^+ to polynomials in the η 's is more complicated. As a first step we must put $(\hat{a}_2^+)^{\sigma}$ in a convenient form. The expression (46.7) suggests that we can write

$$(a_2^+)^{\sigma} = \sum_{n=0}^{\sigma} \eta_2^{\sigma-n} (2, 0)^n R_n^{\sigma}(\hat{N}) \xi_2^n, \quad (47.7)$$

where $R_n^{\sigma}(\hat{N})$ is some function of the number operator alone. In fact for $\sigma = 1$ we get from (46.7) that

$$R_0^1(\hat{N}) = 1, \quad R_1^1(\hat{N}) = -(2\hat{N} + 5)^{-1}. \quad (47.8)$$

We shall prove (47.7) by induction, getting a recursion relation for the $R_n^{\sigma}(\hat{N})$ which we can solve, and thus determining it explicitly. We note that

$$(a_2^+)^{\sigma+1} = [\eta_2 - (2, 0)(2\hat{N} + 5)^{-1}\xi_2] \times \sum_n \eta_2^{\sigma-n} (2, 0)^n R_n^{\sigma}(\hat{N}) \xi_2^n. \quad (47.9)$$

Developing this result and making use repeatedly of the relations

$$\xi_2 R_n^{\sigma}(\hat{N}) = R_n^{\sigma}(\hat{N} + 1)\xi_2, \quad \eta_2 R_n^{\sigma}(\hat{N}) = R_n^{\sigma}(\hat{N} - 1)\eta_2, \quad (47.10)$$

for arbitrary functions of the number operator \hat{N} , we obtain that

$$\begin{aligned} (a_2^+)^{\sigma+1} &= \sum_{n=0}^{\sigma} \eta_2^{\sigma+1-n} (2, 0)^n R_n^{\sigma}(\hat{N}) \\ &\quad \times [1 - 2n(2\hat{N} + 2\sigma + 2n + 3)^{-1}] \xi_2^n \\ &\quad - \sum_{n=1}^{\sigma+1} \eta_2^{\sigma+1-n} (2, 0)^n (2\hat{N} + 2\sigma + 2n + 3)^{-1} \\ &\quad \times R_{n-1}^{\sigma}(\hat{N} + 1) \xi_2^n, \end{aligned} \quad (47.11)$$

which leads to the recursion relation

$$\begin{aligned} (2\hat{N} + 2\sigma + 2n + 3) R_n^{\sigma+1}(\hat{N}) \\ = (2\hat{N} + 2\sigma + 3) R_n^{\sigma}(\hat{N}) - R_{n-1}^{\sigma}(\hat{N} + 1), \end{aligned} \quad (47.12)$$

satisfied by

$$R_n^{\sigma}(\hat{N}) = (-1)^n \binom{\sigma}{n} \frac{(2\hat{N} + 2\sigma + 1)!!}{(2\hat{N} + 2\sigma + 2n + 1)!!}. \quad (47.13)$$

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As $R_n^1(\hat{N}), n = 0, 1$ gives precisely (47.8) we have the $R_n^{\sigma}(\hat{N})$ we require.

We can now write the state (47.6) in the form

$$|\kappa\ell L\rangle = \sum_n \eta_2^{\sigma-n} (2, 0)^n R_n^{\sigma}(\hat{N}) \xi_2^{\tau+n} |3\ell + 3\tau, \ell + \tau, 0\rangle. \quad (47.14)$$

Applying ξ_2 as the derivative $\partial/\partial\eta_{-2}$ and noting that

$$\frac{\partial}{\partial\eta_{-2}} (2, 0) = 2(1, 2), \quad (47.15a)$$

$$\frac{\partial}{\partial\eta_{-2}} (3, 0) = 3(2, 2), \quad (47.15b)$$

$$\frac{\partial(1, 2)}{\partial\eta_{-2}} = \frac{\partial(2, 2)}{\partial\eta_{-2}} = 0, \quad (47.15c)$$

we obtain finally that

$$\begin{aligned} |\kappa\ell L\rangle &= \sum_{r,n} \left\{ C_{rn}^{\sigma\tau\ell} (1, 2)^{\sigma+\tau-n} (2, 2)^n \right. \\ &\quad \times (2, 0)^{3\tau-\tau+n} (3, 0)^{\ell+\tau-2r-n} \Big\} |0\rangle, \end{aligned} \quad (47.16)$$

where the constants $C_{rn}^{\sigma\tau\ell}$ have the form

$$\begin{aligned} C_{rn}^{\sigma\tau\ell} &= B_r^{\ell+\tau} 2^{\tau-n} 3^n \frac{(3r)!(\ell+\tau-2r)!}{(\ell+\tau-2r-n)!} \\ &\quad \times \sum_s 2^s \binom{\tau+s}{n} \frac{R_s^{\sigma}(3\ell+2\tau-s)}{(3\tau-\tau+n-s)!} \\ &= \frac{3^n \sigma! \kappa! (-1)^r 2^r (2\ell+2\tau-2r)!(3r)!}{2^{\ell+n} n! (2\kappa+1)! r! (\ell+\tau-r)! (\ell+\tau-n-2r)!} \\ &\quad \times \sum_s \frac{(-1)^s 4^s (\tau+s)! (2\kappa+1-2s)!}{s! (\sigma-s)! (\tau-n+s)! (3r-\tau+n-s)! (\kappa-s)!}, \end{aligned} \quad (47.17)$$

as $B_r^{\ell+\tau}$ and $R_s^{\sigma}(3\ell+2\tau-s)$ are in turn given by (47.5) and (47.13).

We have thus obtained $|\kappa\ell L\rangle$ for L even as the expression (47.16) in the elementary permissible polynomials (epd) of the η 's. We can also express by (47.16) the states $|\kappa\ell L\rangle$ as polynomials in the creation operators

$$\eta_m = \frac{1}{\sqrt{2}} (\alpha_m - i\pi_m) = \frac{1}{\sqrt{2}} \left(\alpha_m - \frac{\partial}{\partial\alpha^m} \right) \quad (47.18)$$

acting on the ground state $|0\rangle$ of (45.1), but our final purpose is to obtain the state $|\kappa\ell L\rangle$ as a function of the $\alpha_m, m = 2, 1, 0, -1, 2$, and, in the next section, give it in terms of the variables $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$.

In view of the differential character of the operator η_m of (47.18) this seems, at first sight, very difficult to achieve, but it proves very simple thanks to a result due to Dragt [15] which we shall proceed to prove in a way different from the one he followed.

We first shall note that the generators $\mathcal{L}_{mm'}$ of $O(5)$, as well as the generators L_q , $q = 1, 0, -1$ of $O(3)$ have the same form in terms of the η_m and ξ_m (where the latter are interpreted in the differential operator form $\partial/\partial\eta^m$ of (45.4)) as in terms of α_m and $\partial/\partial\alpha^m$.

Remembering the definition (46.3) of $\mathcal{L}_{mm'}$ in terms of $\eta_m, \xi_{m'}$ as well as the form (47.18) of the latter in terms $\alpha_m, \pi_{m'}$ and the fact, indicated in (43.18) that $\pi_m = -i\partial/\partial\alpha^m$ we obtain finally

$$\mathcal{L}_{mm'} = (1/\sqrt{2}) \left\{ \alpha_m \frac{\partial}{\partial\alpha^{m'}} - \alpha_{m'} \frac{\partial}{\partial\alpha^m} \right\}. \quad (47.19)$$

Thus it could be derived immediately from (46.3) if we replace

$$\eta_m \rightarrow \alpha_m, \quad \xi_m = \frac{\partial}{\partial\eta^m} \rightarrow \frac{\partial}{\partial\alpha^m}. \quad (47.20)$$

Turning now our attention to the generators of $O(3)$ given (45.7) we see, using some symmetry properties of the $3j$ coefficients [9], that they could be expressed as

$$\begin{aligned} \hat{L}_q &= (-1)^q \sqrt{15} \sum_{m,m'} \begin{pmatrix} 2 & 2 & 1 \\ m & m' & -q \end{pmatrix} \\ &\times \left[\frac{1}{\sqrt{2}} (\eta_m \xi_{m'} - \eta_{m'} \xi_m) \right]. \end{aligned} \quad (47.21a)$$

As the last square bracket is just $\mathcal{L}_{mm'}$ of (46.3), which has also the form (47.19), we see that \hat{L}_q can be written as

$$\begin{aligned} \hat{L}_q &= (-1)^q \sqrt{15} \sum_{m,m'} \begin{pmatrix} 2 & 2 & 1 \\ m & m' & -q \end{pmatrix} \\ &\times \left[\frac{1}{\sqrt{2}} (\alpha_m \frac{\partial}{\partial\alpha^{m'}} - \alpha_{m'} \frac{\partial}{\partial\alpha^m}) \right]. \end{aligned} \quad (47.21b)$$

Thus the Casimir operators \mathcal{L}^2 of (46.4) takes the form

$$\begin{aligned} \mathcal{L}^2 &= \left(\sum_{m=-2}^2 \alpha_m \frac{\partial}{\partial\alpha_m} \right) \left(\sum_{m=-2}^2 \alpha_m \frac{\partial}{\partial\alpha_m} + 3 \right) \\ &- \left(\sum_{m=-2}^2 \alpha^m \alpha_m \right) \left(\sum_{m=-2}^2 \frac{\partial^2}{\partial\alpha^m \partial\alpha_m} \right), \end{aligned} \quad (47.22)$$

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while the operators L_1 and L_0 of (45.7) associated with the angular momentum can be written as

$$\hat{L}_1 = - \sum_{m=-2}^2 [(1/2)(3+m)(2-m)]^{\frac{1}{2}} \alpha_{m+1} \frac{\partial}{\partial\alpha_m}, \quad (47.23a)$$

$$\hat{L}_0 = \sum_{m=-2}^2 m \alpha_m \frac{\partial}{\partial\alpha_m}. \quad (47.23b)$$

Thus finding a set of polynomials $P_{\kappa\ell L}(\alpha_m)$, function now of α_m , that satisfy the equations

$$\mathcal{L}^2 P_{\kappa\ell L}(\alpha_m) = \kappa(\kappa+3)P_{\kappa\ell L}(\alpha_m), \quad (47.24a)$$

$$\hat{L}_1 P_{\kappa\ell L}(\alpha_m) = 0, \quad (47.24b)$$

$$\hat{L}_0 P_{\kappa\ell L}(\alpha_m) = LP_{\kappa\ell L}(\alpha_m), \quad (47.24c)$$

is a problem that, mathematically, is exactly equal to the one we solved to get the $P_{\kappa\ell L}(\eta_m)$ of (47.16), with the epd (ν, L) appearing there given by (45.10) and (45.20) in terms of the creation operators η_m .

Thus it is immediately clear that $P_{\kappa\ell L}(\alpha_m)$ satisfying Eq. (47.24) has the form

$$\begin{aligned} P_{\kappa\ell L}(\alpha_m) &= \sum_{r,n} \left[C_{rn}^{\sigma\tau\ell} \{1,2\}^{\sigma+\tau-n} \{2,2\}^n \right. \\ &\quad \left. \{2,0\}^{3r-\tau+n} \{3,0\}^{\ell+\tau-2r-n} \right], \end{aligned} \quad (47.25)$$

with $C_{rn}^{\sigma\tau\ell}$ given by (47.17) and the $\{\nu, L\}$ are the one of the type defined in (47.3).

The question that remains though is what is the complete form in terms of the α_m of the ket $|\kappa\ell L\rangle$ obtained in (47.16) as the operator $P_{\kappa\ell L}(\eta_m)$ acting on the ground state of (45.1). For this we note that from (44.21), L_1, L_0 are functions of the Euler angles $\vartheta_1, \vartheta_2, \vartheta_3$ and their derivatives. On the other hand the Casimir operator \mathcal{L}^2 of (47.22) can only be a function of $\gamma, \vartheta_1, \vartheta_2, \vartheta_3$ and their derivatives as it can not depend on the radial coordinate β , or $\partial/\partial\beta$, in the same way that, for the three-dimensional oscillator, the Casimir operator \hat{L}^2 of $O(3)$ depends on θ, φ and their derivatives, but not on r or $\partial/\partial r$. Thus clearly $P_{\kappa\ell L}(\alpha_m)$ is a solution of our problem in terms of the variables α_m , up to some function of β only, that necessarily is an eigenfunction with eigenvalue 0 of the Casimir operators \mathcal{L}^2, L^2, L_0 of the $O(5) \supset O(3) \supset O(2)$ chain of groups.

To find this function we need only to compare a particular case of $|\kappa\ell L\rangle$ of (47.16) with the corresponding $P_{\kappa\ell L}(\alpha_m)$, and the simplest one is when $\kappa = \ell = L = 0$, in which

$$|000\rangle = \frac{1}{2}\pi^{-5/4} \exp(-\beta^2/2), \quad (47.26a)$$

$$P_{000}(\alpha_m) = 1. \quad (47.26b)$$

Clearly then, except for a difference in the normalization constant, we have that, as a function of the α_m , the ket $|\kappa\ell L\rangle$ of (47.16) becomes

$$|\kappa\ell L\rangle = P_{\kappa\ell L}(\alpha_m) \exp \left[\left(\sum_{m=-2}^2 \alpha_m \alpha^m \right) / 2 \right], \quad (47.27)$$

where we used the definition (44.2) of β^2 .

If we want now the full expression of the states of the five-dimensional oscillator as functions of the variables α_m , this can be written, up to a normalization constant, as the ket

$$|\nu\kappa\ell LM\rangle = L_j^{\kappa+3/2}(\beta^2) \exp(-\beta^2/2) \left[\hat{L}_{-1}^{L-M} P_{\kappa\ell L}(\alpha_m) \right], \quad (47.28)$$

where $\nu = 2j + \kappa$ or, equivalently $j = (\nu - \kappa)/2$, $L_j^{\kappa+\frac{3}{2}}(\beta^2)$ is a Laguerre polynomial of the order indicated, and \hat{L}_{-1} is the operator (47.21) when $q = -1$, and which we need to apply to $P_{\kappa\ell L}(\alpha_m)$ to give the appropriate projection M to the angular momentum.

Some of the values appearing in the ket (47.28) correspond respectively to the indices that characterize the irreducible representation of the chain of groups

$$U(5) \supset O(5) \supset O(3) \supset O(2) \quad (47.29a)$$

$$\nu \quad \kappa \quad L \quad M, \quad (47.29b)$$

as indicated below each one of them. There is though an extra index ℓ that characterizes the number of triplets $\{3, 0\}$ in the α_m that have angular momentum 0, and are required to distinguish irreps L of $O(3)$ that appear more than once in an irrep κ of $O(5)$. Thus our basis $|\nu\kappa\ell LM\rangle$, while orthogonal in the indices ν, κ, L, M does not have this property for the ℓ . The whole basis could though be orthonormalized in the full set of indices by a Hilbert-Schmidt procedure [18], or, more elegantly, by applying to the basis (47.28) an hermitian operator, function of the generators of $O(5)$, that would be scalar in $O(3)$, as was done in the case $U(3) \supset O(3)$ in Eq. (38.46).

We now proceed to express the kets (47.28) as functions of the variables $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$.

48. THE POLYNOMIALS $P_{\kappa\ell L}(\alpha_m)$ AS FUNCTIONS

48 The Polynomials $P_{\kappa\ell L}(\alpha_m)$ as Functions of the Variables $\vartheta_1, \vartheta_2, \vartheta_3, \gamma$ and β and the Determination of $\phi_K^{\kappa\ell L}(\gamma)$

The ket $|\nu\kappa\ell LM\rangle$ of the five-dimensional oscillator, is given in the previous sections of this chapter, in two different forms. One of them appears in Eq. (44.28), but where $\phi_K^{\kappa\ell L}(\gamma)$ is still unknown, and the other where it is expressed explicitly in terms of the α_m in Eq. (47.28) where $P_{\kappa\ell L}(\alpha_m)$ with L even is given by Eq. (47.25) in terms of appropriate epd of the α_m . As the form (44.28) of the ket $|\nu\kappa\ell LM\rangle$ is the more convenient one for calculations of matrix elements of Hamiltonians, or of transition probabilities, as will be seen in the following sections, we should make use of Eq. (47.28) to determine the $\phi_K^{\kappa\ell L}(\gamma)$ appearing in (44.28), as in this last equation $F_j^\kappa(\beta)$ of (44.31) and $D_{MK}^{L*}(\vartheta_i)$ of Eq. (4.12) p. 52 of Rose's book [9] are well known.

For our purpose we can limit ourselves to the ket

$$|\nu = \kappa, \kappa, \ell, L, M = L\rangle \equiv |\kappa\ell L\rangle = [\beta^{-\kappa} P_{\kappa\ell L}(\alpha_m)] \beta^\kappa \exp(-\beta^2/2), \quad (48.1)$$

and comparing it with (44.28) we arrive, after eliminating the common factor $\beta^\kappa \exp(-\beta^2/2)$ that it has with (48.1), to the relation

$$\begin{aligned} & \sum_K \phi_K^{\kappa\ell L}(\gamma) \left[D_{LK}^{L*}(\vartheta_i) + D_{L-K}^{L*}(\vartheta_i) \right] \\ &= \sum_n \left[\{1, 2\}/\beta \right]^{\sigma+\tau-n} \left[\{2, 2\}/\beta^2 \right]^n f_n^{\sigma\tau\ell}(x). \end{aligned} \quad (48.2)$$

The terms appearing in Eq. (48.2) have the following definition:

$$\left[\{1, 2\}/\beta \right] = (\alpha_2/\beta), \quad (48.3a)$$

$$\left[\{2, 2\}/\beta^2 \right] = \sqrt{7}\beta^{-2}[\alpha \times \alpha]_2^2, \quad (48.3b)$$

where the \times sign indicates angular momentum coupling of the α 's to $L = M = 2$ as in (45.10). From (47.25) and (47.3b) we see that

$$f_n^{\sigma\tau\ell}(x) = \sum_r (-\sqrt{2})^{\ell+\tau-2r-n} C_{rn}^{\sigma\tau\ell} x^{\ell+\tau-2r-n}, \quad (48.4)$$

with the numerical coefficient $C_{rn}^{\sigma\tau\ell}$ given by (47.17) and $x = \cos 3\gamma$ as in (47.4). Note that σ, τ are related to κ, ℓ, L through (46.18).

To obtain $\phi_K^{\kappa\ell L}(\gamma)$ through (48.2) we need to write powers of the expressions (48.3a,b) in terms of the functions $D_{LK}^{L*}(\vartheta_i)$. For this purpose we note that from the definitions (48.3) and the relation (44.1) we have

$$\begin{aligned}\beta^{-1}\{1, 2\} &= (\alpha_2/\beta) \\ &= (1/\sqrt{2}) \left[D_{22}^{2*}(\vartheta_i) + D_{2-2}^{2*}(\vartheta_i) \right] \sin \gamma + D_{20}^{2*}(\vartheta_i) \cos \gamma,\end{aligned}\quad (48.5)$$

$$\begin{aligned}\beta^{-2}\{2, 2\} &= \beta^{-2}\sqrt{7}[\alpha \times \alpha]_2^2 = \sqrt{7} \sum_m D_{2m}^{2*}(\vartheta_i) \beta^{-2}[\alpha \times \alpha]_m^2 \\ &= - \left\{ \left[D_{22}^{2*}(\vartheta_i) + D_{2-2}^{2*}(\vartheta_i) \right] \sin(-2\gamma) + \sqrt{2} D_{20}^{2*}(\vartheta_i) \cos(-2\gamma) \right\},\end{aligned}\quad (48.6)$$

where $[\alpha \times \alpha]_m^2$ indicates the coupling of two a_m of (43.25–27) to total angular momentum 2 and projection m . As we have

$$D_{LK}^{L*}(\vartheta_i) = \exp(iL\vartheta_i) d_{LK}^L(\vartheta_2) \exp(iK\vartheta_3), \quad (48.7)$$

with a well known [9] expression for $d_{LK}^L(\vartheta_2)$, we immediately obtain from (48.5) that

$$[\beta^{-1}\{1, 2\}]^r = \sum_K D_{2r,K}^{2*}(\vartheta_i) S_K^{2r}(\gamma), \quad (48.8)$$

where the function $S_K^{2r}(\gamma)$ takes the form

$$\begin{aligned}S_K^{2r}(\gamma) &= \left[\frac{(2r+K)!(2r-K)!}{(4r)!} \right]^{\frac{1}{2}} \\ &\times \sum_q \left\{ \binom{r}{2q-\frac{K}{2}} \binom{2q-\frac{K}{2}}{q} (\sqrt{6})^r \left(\frac{1}{2\sqrt{3}} \right)^{2q-(K/2)} \right. \\ &\times (\cos \gamma)^{r+(K/2)-2q} (\sin \gamma)^{2q-(K/2)} \Big\} \\ &= \left[\frac{(2r+K)!(2r-K)!}{(4r)!} \right]^{\frac{1}{2}} \frac{r!(\sqrt{6})^r (2\sqrt{3})^{-(K/2)}}{(K/2)![r-(K/2)]!} \\ &\times (\cos \gamma)^{-(K/2)+r} (\sin \gamma)^{(K/2)} \\ &\times {}_2F_1 \left(-\frac{r}{2} + \frac{K}{4}, -\frac{r}{2} + \frac{K}{4} + \frac{1}{2}; \frac{K}{2} + 1; \frac{1}{3} \tan^2 \gamma \right),\end{aligned}\quad (48.9)$$

and in which ${}_2F_1$ is an hypergeometric function and K is restricted to even values. We note also that if we replace K by $-K$ and $2q$ by $2q-K$ in (48.9) we get an identical expression and thus we have the property

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$$S_K^{2r}(\gamma) = S_{-K}^{2r}(\gamma). \quad (48.10)$$

Note that the relatively simple form for $S_K^{2r}(\gamma)$ is due to the fact that in all our analysis we have representations of $O(3)$ where $M = L$, i.e., $D_{LK}^{L*}(\vartheta_i)$, and thus the summation defining $d_{LK}^L(\vartheta_2)$ in Eq. (4.13) of p. 52 in Rose's book [9] reduces to a single term.

From the above results and (48.6) we then immediately see that also

$$[\beta^{-2}\{2, 2\}]^n = (-\sqrt{2})^n \sum_K D_{2n,K}^{2n*}(\vartheta_i) S_K^{2n}(-2\gamma). \quad (48.11)$$

Thus we have that the product

$$[\beta^{-1}\{1, 2\}]^{(L/2)-n} [\beta^{-2}\{2, 2\}]^n = \sum_K G_K^{nL}(\gamma) D_{LK}^{L*}(\vartheta_i), \quad (48.12)$$

where

$$\begin{aligned}G_K^{nL}(\gamma) &= (-\sqrt{2})^n \sqrt{2L+1} \sum_{K', K''} \left\{ \binom{L-2n}{K'} \binom{2n}{K''} \binom{L}{-K} \right. \\ &\times S_{K'}^{L-2n}(\gamma) S_{K''}^{2n}(-2\gamma) \Big\}.\end{aligned}\quad (48.13)$$

In (48.13) we have an ordinary $3j$ symbol of $O(3)$ and in deriving the result we made only use of the well known decomposition of products [9] of $D_{MK}^{L*}(\vartheta_i)$.

Remembering that we are discussing the case when L is even we see, from (48.10) and the symmetry properties of the $3j$ symbols coefficients [9], that

$$G_K^{nL}(\gamma) = G_{-K}^{nL}(\gamma). \quad (48.14)$$

Introducing now (48.12) in to (48.2), we obtain

$$\phi_K^{\kappa\ell L}(\gamma) = \sum_n G_K^{nL}(\gamma) f_n^{\sigma\tau\ell}(x), \quad (48.15)$$

where $G_K^{nL}(\gamma)$ is the completely defined function of γ of (48.13) while $f_n^{\sigma\tau\ell}(x)$ is given by (48.4) with $x = \cos 3\gamma$ and σ, τ related to κ, ℓ, L by (46.18).

As we are only discussing here the case of L even, the symmetry relation (48.14) for G_K^{nL} , was sufficient in establishing the formula (48.15) for $\phi_K^{\kappa\ell L}(\gamma)$ through the relation (48.2).

Note that from the relation (48.14) and the definitions (48.15) we have for L even the symmetry properties

$$\phi_K^{\kappa\ell L}(\gamma) = \phi_{-K}^{\kappa\ell L}(\gamma), \quad (48.16)$$

and thus the state (44.28) can be written as

$$|\nu\kappa\ell LM\rangle = F_j^\kappa(\beta) \sum_K \phi_K^{\kappa\ell L}(\gamma) D_{MK}^{L*}(\vartheta_i), \quad (48.17)$$

with K restricted to the values given in (44.30) and $2j + \kappa = \nu$.

A similar expression for the $\phi_K^{\kappa\ell L}(\gamma)$ when L is odd will be established in the section 51. Our main point though is that with the explicit form of $\phi_K^{\kappa\ell L}(\gamma)$ in (48.15), we see from (44.28) that we have determined the ket $|\nu\kappa\ell LM\rangle$ of the five-dimensional oscillator characterized by the chain of groups $U(5) \supset O(5) \supset O(3) \supset O(2)$, whose irreps correspond respectively to ν, κ, L, M , and where we have the extra multiplicity index ℓ .

While our algebraic expression for $\phi_K^{\kappa\ell L}(\gamma)$ are complicated, a program has been elaborated by Yannouleas and Pacheco [19] that allows us to determine them explicitly by computer, and thus make them available for physical applications.

49 Operators for Hamiltonians and Transition Probabilities for the Collective Model of the Nucleus and Their Matrix Elements

If we use the units $\hbar = B_2 = C_2 = 1$ of (43.16) then the Hamiltonian that includes separately only quadratic terms in π_m and α_m , and is, as it should, invariant under rotations in space, can only have the form H of (43.17), i.e., that of an harmonic oscillator of five dimensions, whose eigenvalues are $\nu + (5/2)$, and eigenstates the kets $|\nu\kappa\ell LM\rangle$ that we have discussed in the previous section.

Because of the simplicity of the spectra, and the lack of more free parameters, H is not by itself a useful Hamiltonian to discuss collective motions. It does have though the advantage of providing us with a complete set of eigenstates in terms of the collective variables α_m , or, equivalently, in terms of $\vartheta_1, \vartheta_2, \vartheta_3, \gamma, \beta$. Thus we would like to consider more general Hamiltonians \mathcal{H} than those of the five-dimensional oscillator H , but keep the latter as a starting point in the calculations and use its eigenstates to get the matrix representation of \mathcal{H} , to be used later in variational procedures to determine eigenvalues of \mathcal{H} which can then be compared with experimental results.

The observations of the previous paragraph suggest an \mathcal{H} of the form

$$\mathcal{H} = H + K(\alpha_m, \pi_m) + V(\alpha_m), \quad (49.1)$$

where, because of (43.16), H is given by (43.17) while $K(\alpha_m, \pi_m)$ and $V(\alpha_m)$ are respectively additions to the kinetic and potential energy of the oscillator that are polynomial functions of the variables indicated. Both K and V should be scalar, hermitian and invariant under parity transformation. The last condition is automatically satisfied as α_m, π_m are second order Racah tensors of positive parity, and the scalar property can be achieved by coupling the α_m, π_m appearing in K and V , to total angular momentum zero.

The $K(\alpha_m, \pi_m)$ should be of second degree in the π_m , as the kinetic energy of the oscillator itself is $(1/2) \sum_m (\pi_m \pi^m)$. As a function of the α_m we have, in principle, no limitation to their degree but, for reasons of simplicity, we follow Gneuss and Greiner [7] and limit them to the second one. Without loss of generality [20] we could then limit K to the form

$$K(\alpha_m, \pi_m) = B_3 \{[\pi \times \alpha]^2 \times \pi\}^0 + B_4 \{[\pi \times \pi]^0 \times [\alpha \times \alpha]^0\}^0, \quad (49.2)$$

with an appropriate symmetrization to make them hermitian.

We shall follow in this section a notation in which the multiplication sign \times indicates coupling of the angular momenta to the total one indicated at the end of the corresponding parenthesis thus, for example,

$$\{[\pi \times \alpha]^2 \times \pi\}^0 = \sum_{mm'm''} \begin{pmatrix} 2 & 2 & 2 \\ m & m' & m'' \end{pmatrix} \pi_m \alpha_{m'} \pi_{m''}. \quad (49.3)$$

For the $V(\alpha_m)$ there is no problem of hermiticity as it only depends on the α_m that commute among themselves. There is furthermore the need that it should be a scalar, i.e., with total angular momentum $L = 0$. If we then want to get the most general homogeneous polynomial in α_m of degree ν and $L = 0$, we just have to look back to (45.23) and substitute the epd's (ν, L) in the η 's in terms of $\{\nu, L\}$ in the α 's. For $L = 0$ this polynomial depends only on $\{2, 0\}$ and $\{3, 0\}$ and thus the most general $V(\alpha_m)$ can be written as

$$\begin{aligned} V(\alpha_m) &= \sum_{\rho, \ell} (-\sqrt{2})^{-\ell} V_{\rho \ell} \{2, 0\}^\rho \{3, 0\}^\ell \\ &= \sum_{\rho, \ell} V_{\rho \ell} \beta^{2\rho+3\ell} (\cos 3\gamma)^\ell, \end{aligned} \quad (49.4)$$

where $V_{\rho \ell}$ are a set of constants depending on the indices ρ, ℓ which go from 0 to some maximum value of the sum $2\rho + 3\ell$. The right hand side of (49.4) was obtained using the relations (47.3).

To get the basic type of operator whose matrix elements with respect to the states $|\nu\kappa\ell LM\rangle$ we need to evaluate, we note that, up to a normalization constant, we have from (44.33) that

$$\phi_0^{3\ell, \ell, 0}(\gamma) = P_\ell(\cos 3\gamma), \quad (49.5)$$

where P_ℓ is a Legendre polynomial of order ℓ . As x^ℓ can be developed in terms of $P_j(x)$ with $0 \leq j \leq \ell$, we could replace $(\cos 3\gamma)^\ell$ by a linear combination of terms $\phi_0^{3j, j, 0}(\gamma)$ and thus, keeping the notation ℓ rather than j , $V(\alpha_m)$ is a linear combination of operators of the form

$$\beta^{2\rho+3\ell} \phi_0^{3\ell, \ell, 0}(\gamma). \quad (49.6)$$

We turn now our attention to $K(\alpha_m, \pi_m)$ of (49.2) to determine which is the basic operator in this case. The presence of π_m seems at first sight to cause a great problem as it corresponds to the differential operator $-i\partial/\partial\alpha^m$, but this is not the case as from (43.17) we see that

$$-i\pi_m = [H, \alpha_m], \quad (49.7)$$

from the fact that

$$[\pi_m, \alpha^m] = -i\delta_m^m. \quad (49.8)$$

As H is diagonal in the harmonic oscillator basis, it is convenient to replace [21] π_m in $K(\alpha_m, \pi_m)$ by $i[H, \alpha_m]$ and thus we need the matrix elements of the α_m given by (48.5) when we replace the lower index 2 by m . As α_m is "harmonic", i.e., satisfies the equation

$$\mathcal{L}^2 \alpha_m = 4\alpha_m, \quad (49.9)$$

where \mathcal{L}^2 is given by (47.22) it could then also be expressed as

$$\alpha_m = \beta \sum_k \phi_k^{102}(\gamma) D_{mk}^{2*}(\vartheta_i), \quad (49.10)$$

where

$$\phi_{\pm 2}^{102} = (1/\sqrt{2}) \sin \gamma, \quad \phi_{\pm 1}^{102} = 0, \quad \phi_0^{102}(\gamma) = \cos \gamma. \quad (49.11)$$

As we are dealing with several α_m, π_m in the terms in $K(\alpha_m, \pi_m)$, we see from (49.7) that they can be reduced to several α 's, as will be seen in the next section, so finally the type of operator, in terms of which both $K(\alpha_m, \pi_m)$ and $V(\alpha_m)$ can be expressed, can be put in the form

$$\beta^{2\rho+\kappa} \sum_K \phi_K^{\kappa\ell L}(\gamma) D_{MK}^{L*}(\vartheta_i), \quad (49.12)$$

with K restricted to the values (44.30) and $\phi_K^{\kappa\ell L}(\gamma)$ satisfying the symmetry relation (48.16).

So far we have spoken only of Hamiltonians, but if we want to consider quadrupole transition operators Q_m , we can calculate them from the hydrodynamical model [20] to obtain, in dimensionless form, that

$$Q_m = \left(\alpha_m - \frac{10}{\sqrt{70\pi}} [\alpha \times \alpha]_m^2 \right). \quad (49.13)$$

We showed in (49.10) that α_m is a particular case of (49.12) when $\rho = 0$, $\kappa = 1$, $\ell = 0$ and $L = 2$, and from (48.6) we easily see that $\sqrt{7}[\alpha \times \alpha]_m^2$ is also of the form (49.12) but now with $\rho = 0, \kappa = 2, \ell = 0, L = 2$, as it is "harmonic", i.e., an eigenstate of \mathcal{L}^2 of (47.22), and we have from (48.6) that

$$\phi_{\pm 2}^{202}(\gamma) = \sin 2\gamma, \quad \phi_{\pm 1}^{202}(\gamma) = 0, \quad \phi_0^{202} = -\sqrt{2} \cos 2\gamma. \quad (49.14)$$

Thus all the matrix elements we require can be reduced to a linear combination of those in (49.12) with respect to the states $|\nu\kappa\ell LM\rangle$ of (48.17).

We proceed to write this matrix element explicitly, making use of the integral over the Euler angles of three $D_{MK}^L(\vartheta_i)$ functions given in (4.62) of p. 75 of Rose's book [9] and the fact that $\phi_K^{\kappa\ell L}(\gamma)$, as derived in the previous section, are real and satisfy the symmetry relations (48.16). Thus we get

$$\begin{aligned} & \langle \nu'' \kappa'' \ell'' L'' M'' | \beta^{2\rho+\kappa} \sum_K \phi_K^{\kappa\ell L}(\gamma) D_{MK}^{L*}(\vartheta_i) | \nu' \kappa' \ell' L' M' \rangle \\ &= (8\pi^2) \left[\int_0^\infty F_{j''}^{\kappa''}(\beta) \beta^{2\rho+\kappa} F_{j'}^{\kappa'}(\beta) \beta^4 d\beta \right] (-1)^{M''} \begin{pmatrix} L & L' & L'' \\ M & M' & -M'' \end{pmatrix} \\ & \times \int_0^{\frac{\pi}{2}} \sum_{KK'K''} \begin{pmatrix} L & L' & L'' \\ K & K' & K'' \end{pmatrix} \phi_K^{\kappa\ell L}(\gamma) \phi_{K'}^{\kappa'\ell' L'}(\gamma) \phi_{K''}^{\kappa''\ell'' L''}(\gamma) \sin 3\gamma d\gamma \\ &= \left\{ \left[j'! \Gamma(j' + \kappa' + \frac{5}{2}) \right]^{-\frac{1}{2}} \left[j''! \Gamma(j'' + \kappa'' + \frac{5}{2}) \right]^{-\frac{1}{2}} (-1)^{j'+j''} \right. \\ & \times \frac{\Gamma\left[\frac{1}{2}(2\rho+\kappa+\kappa'+\kappa''+5)\right] \Gamma\left[\frac{1}{2}(2\rho+\kappa-\kappa'+\kappa'')+1\right] \Gamma\left[\frac{1}{2}(2\rho+\kappa+\kappa'-\kappa'')+1\right]}{\Gamma\left[\frac{1}{2}(2\rho+\kappa-\kappa'+\kappa'')-j'+1\right] \Gamma\left[\frac{1}{2}(2\rho+\kappa-\kappa'+\kappa')-j''+1\right]} \\ & \times {}_3F_2 \left[\begin{matrix} \frac{1}{2}(2\rho+\kappa+\kappa'+\kappa''+5), -j', -j'' \\ \frac{1}{2}(2\rho+\kappa-\kappa'+\kappa'')-j'+1, \frac{1}{2}(2\rho+\kappa+\kappa'-\kappa'')-j''+1 \end{matrix}; 1 \right] \\ & \times (8\pi^2)(-1)^{M''} \begin{pmatrix} L' & L & L'' \\ M' & M & -M'' \end{pmatrix} (\kappa\ell L, \kappa'\ell' L', \kappa''\ell'' L''). \end{aligned} \quad (49.15)$$

In the right hand side of (49.15) the curly bracket corresponds to the value of the integral with respect to the variable β that is given explicitly in reference [22] in terms of gamma and hypergeometric functions, in which, as indicated in (44.29), we have

$$j' = (1/2)(\nu' - \kappa'), \quad j'' = (1/2)(\nu'' - \kappa''). \quad (49.16)$$

The round bracket of two rows in the standard $3j$ symbol, with the upper row indicating the angular momenta $L'L''L''$ and the lower one their projections, and its appearance is due to the Wigner–Eckart theorem of p. 88 of reference [9].

The last single line round bracket in Eq. (49.15) is a short hand notation for the integral with respect to γ that appears also in the same equation, and which we shall rewrite explicitly because of its importance in the calculations

$$\begin{aligned} & (\kappa L, \kappa' \ell' L', \kappa'' \ell'' L'') \\ &= \int_0^{\frac{\pi}{3}} \sum_{KK'K''} \left[\begin{pmatrix} L & L' & L'' \\ K & K' & K'' \end{pmatrix} \phi_K^{\kappa L}(\gamma) \right. \\ & \quad \times \left. \phi_{K'}^{\kappa' \ell' L'}(\gamma) \phi_{K''}^{\kappa'' \ell'' L''}(\gamma) \sin 3\gamma \right] d\gamma. \end{aligned} \quad (49.17)$$

Its mathematical meaning is that of a reduced Wigner coefficient in the chain of groups $O(5) \supset O(3)$, and its numerical determination can be obtained in principle from the explicit expression of Eqs. 4, 13 and 15 of section 48 for $\phi_K^{\kappa L}(\gamma)$. This of course is very complicated algebraically, but can be done straightforwardly in a computer as all the resulting integrals are elementary. The computer analysis has in fact been carried out by Yannouleas and Pacheco [23] and Hess *et al.* [24], and the interested reader should consult these last papers both for orthonormalization procedure for the function $\phi_K^{\kappa L}(\gamma)$ as well as for the numerical determination of the matrix elements (49.15).

With present computing facilities it is perfectly feasible to use the procedures discussed in this chapter to derive the matrix elements with respect to the states (48.17) of the Hamiltonian of (49.1), choosing appropriately the coefficients B_3, B_4 in (49.2) and $V_{\rho\ell}$ in (49.4), so as to get the best fit to levels of particular nuclei. In fact this type of program has been carried out by Hess *et al.* [25], and we shall discuss some of his results in the next section.

50 Applications to Quadrupole Collective Motions in Nuclei

In the preceding sections of this chapter we have developed all the formalism required for quadrupole collective motions, based on properties of eigenstates of the five-dimensional oscillator, as well as on operators depending on its variables α_m , $m = 2, 1, 0, -1, -2$, or $\vartheta_1, \vartheta_2, \vartheta_3, \gamma$ and β and the corresponding conjugate momenta.

In this section we wish to apply them to specific nuclei and we shall choose, in particular, ^{238}U , as in the work of Hess *et al.* [25] the formalism presented in this chapter, based mainly on the work of Chacón and Moshinsky [11,16], was extensively used.

In the present section we shall consider three subjects, to be designated as **a**, **b**, **c**, dealing respectively with the potential energy surfaces, the kinetic energy and the actual application to energy levels and transition probabilities in ^{238}U .

a) Potential energy surfaces associated with $V(\alpha_m)$

According to Eq. (49.4) the potential $V(\alpha_m)$ is a function of powers of β, γ as polar coordinates and $a_0, \sqrt{2}a_2$, defined in (43.26), as the corresponding cartesian ones. Because of symmetry considerations [8] γ can be restricted to the interval $0 \leq \gamma \leq \frac{\pi}{3}$, and thus $a_0, \sqrt{2}a_2$ are positive, *i.e.*, appear only in the first quadrant. In the following figures we will take a_0 as the abscissa and $\sqrt{2}a_2$ as the ordinate, with both being positive.

Our potential $V(\alpha_m)$ is actually a function of only β, γ , *i.e.*, $V(\beta, \gamma)$ or, equivalently of $a_0, \sqrt{2}a_2$. If the coefficients $V_{\rho\ell}$ are selected, this potential has a definite value at each point (β, γ) or $(a_0, \sqrt{2}a_2)$ and, if we connect by a curve all points that have a definite value of V , we get what is called Potential Energy Surfaces (PES), as seen in Fig. IX.1.

From a classical standpoint, the form of the liquid drop for a definite set of parameters $V_{\rho\ell}$, and in the frame of reference fixed in the body, will be given by the values of β, γ for which the potential $V(\beta, \gamma)$ has a minimum.

To discuss this form we note that from relations (43.24) and (43.26) we obtain

$$\frac{1}{\sqrt{2}}\beta \sin \gamma = \frac{1}{2}\sqrt{\frac{8\pi}{15}}(\alpha'_{xx} - \alpha'_{yy}), \quad (50.1a)$$

$$\beta \cos \gamma = \sqrt{\frac{8\pi}{15}} \frac{1}{\sqrt{6}}(2\alpha'_{zz} - \alpha'_{xx} - \alpha'_{yy}). \quad (50.1b)$$

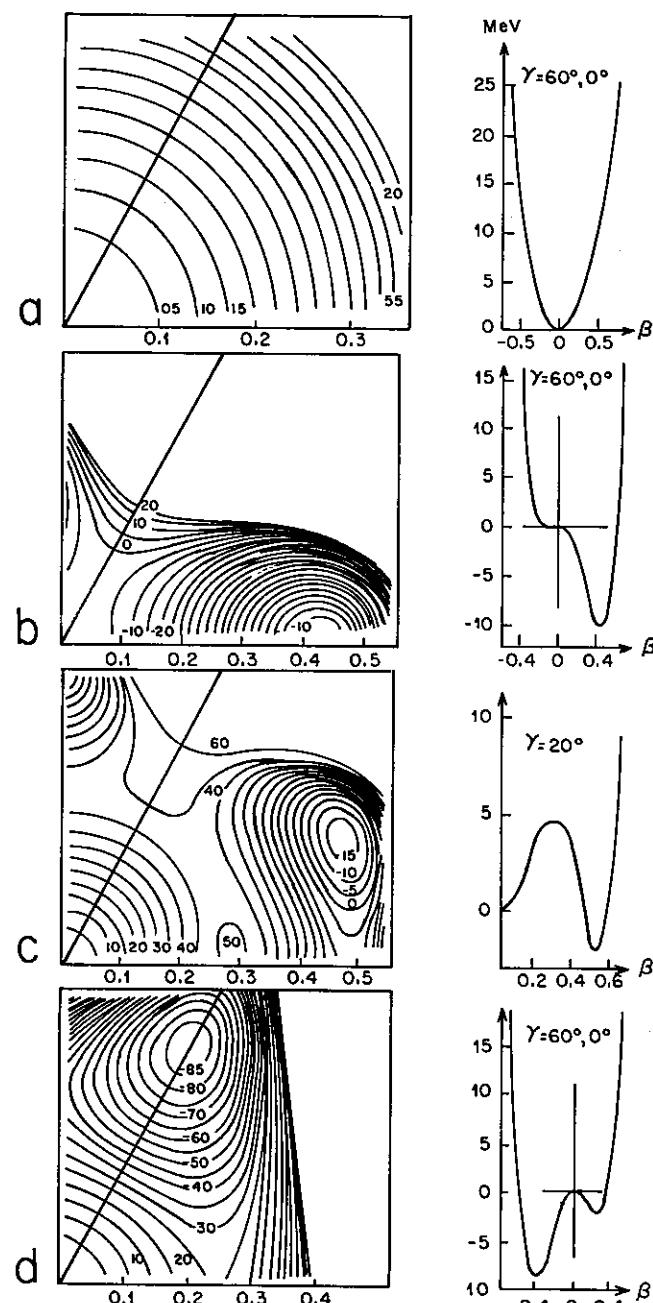


Figure IX.1. Three different types of Potential Energy Surfaces (PES). The first one is a PES of a harmonic oscillator, the second and fourth one of a rotator (prolate and oblate respectively) and the third one of a triaxial nucleus (P. O. Hess *et al.*,

If the minimum occurs when $\beta = 0$, then from (50.1) we see that $\alpha'_{zz} = \alpha'_{yy} = \alpha'_{zz}$ and from (43.24) the form would be spherical as indicated in Fig. IX.1a. A potential having this property could be the one of the harmonic oscillator, *i.e.*, proportional to β^2 , as illustrated in the curve adjoining Fig. IX.1a.

If the minimum occurs when $\beta \neq 0$ but $\gamma = 0^\circ$ then from (50.1a) we have $\alpha'_{zz} = \alpha'_{yy}$ and $\beta = (16\pi/45)^{1/2}(\alpha'_{zz} - \alpha'_{xx})$. From (43.24) we see that we have an ellipsoid of revolution which, because $\beta > 0$, it is prolate, *i.e.*, cigar shaped. This situation is illustrated in Fig. IX.1b where on its right hand side we give the possible form of the potential as function β , when $\gamma = 60^\circ$ and $\gamma = 0^\circ$.

If the minimum occurs when both β and γ are different from 0, then from (50.1) we see that $\alpha'_{zz} \neq \alpha'_{xx} \neq \alpha'_{yy}$ and we have a triaxial nucleus. This is illustrated in Fig. IX.1c, where the minimum appears at $\gamma = 20^\circ$, and on its right hand side we give the possible form of the potential as function of β when $\gamma = 20^\circ$.

Finally if the minimum occurs when $\gamma = 60^\circ$, it is best to analyze the situation when $\gamma = 180^\circ$ where the behavior is repeated according to Fig. 4 in Chapter 4 of reference [8]. In that case we see from (50.1) that the relations are the same as those appearing in our discussion of the case when $\gamma = 0^\circ$ but with β replaced by $-\beta$, so we have an oblate ellipsoid of revolution, *i.e.*, disc shaped. This situation is illustrated in Fig. IX.1d, where on its right hand side we give the possible form of the potential when $\gamma = 60^\circ$ and $\gamma = 0^\circ$.

When we are discussing a particular nucleus, the parameter have to be fixed by a mean square approach to the energy levels. Once they are known, figures of the type of Fig. IX.1 can be drawn and thus, according to the place where the minimum appears, we can speak of the nucleus as spherical, prolate, triaxial or oblate. Examples of this type are given in Figs. 10 and 11 of Chapter 8 of reference [8], and later on will also be presented here when we discuss the nucleus ^{238}U .

b) Reduction of the matrix elements of the kinetic energy type to those discussed in (45.15)

In Eq. (49.2) we indicated that for the kinetic energy, besides terms of the harmonic oscillator type $\sum_m (\pi_m \pi^m)$, we would have others that involve both the momenta π_m and the coordinates α_m .

We indicated in (49.7), how it would be possible to replace π_m by the commutator of α_m with the Hamiltonian H of the harmonic oscillator. This property could serve us well to reduce the matrix elements of kinetic energy

terms, to those of the type (49.15) for which extensive programs have been developed [23,24].

We shall start by introducing the compact notation ν for the set of numbers that characterize the eigenstates we discussed in the previous section, i.e.,

$$|\nu\rangle \equiv |\nu\kappa\ell LM\rangle. \quad (50.2)$$

Using then (49.7) and the fact that the ket $|\nu\rangle$ is an eigenstate of H with eigenvalue $(\nu + \frac{5}{2})$, we have the following relation between matrix elements [21]:

$$\begin{aligned} \langle\nu'|\pi_m|\nu\rangle &= i\langle\nu'|H\alpha_m - \alpha_m H|\nu\rangle \\ &= i(\nu' - \nu)\langle\nu'|\alpha_m|\nu\rangle = (-1)^{\frac{\nu'-\nu}{2}}\langle\nu'|\alpha_m|\nu\rangle. \end{aligned} \quad (50.3)$$

The last result in (50.3) comes out of the fact that from (43.19) the matrix of α_m has the selection rule $\nu' = \nu \pm 1$ and so $i(\nu' - \nu)$ can be expressed as the phase indicated in (50.3).

Let us now turn to the kinetic energy term in Eq. (49.3). It is easily seen that it is already hermitian so we just have to calculate the matrix element [20]:

$$\begin{aligned} \langle\nu'|\{[\pi \times \alpha]^2 \times \pi\}^0|\nu\rangle &= \sum_{mm'm''} \left\{ \begin{pmatrix} 2 & 2 & 2 \\ m & m' & m'' \end{pmatrix} \right. \\ &\quad \times \sum_{\nu_1 \nu_2} \langle\nu'|\pi_m|\nu_1\rangle \langle\nu_1|\alpha_{m'}|\nu_2\rangle \langle\nu_2|\pi_{m''}|\nu\rangle \Big\} \\ &= \sum_{mm'm''} \left\{ \begin{pmatrix} 2 & 2 & 2 \\ m & m' & m'' \end{pmatrix} \sum_{\nu_1, \nu_2} (-1)^{\frac{\nu'-\nu_1}{2}} (-1)^{\frac{\nu_2-\nu}{2}} \right. \\ &\quad \times \langle\nu'|\alpha_m|\nu_1\rangle \langle\nu_1|\alpha_{m'}|\nu_2\rangle \langle\nu_2|\alpha_{m''}|\nu\rangle \Big\}, \end{aligned} \quad (50.4)$$

where we have introduced the complete set of intermediate states characterized by ν_1 and ν_2 as in (50.2), and used (50.3).

We now have to analyze separately the different relations between ν' and ν due to the selection rule $\nu' = \nu \pm 1$ for just one of the α_m operators. Clearly, from the appearance of the three matrix elements of the α 's in (50.4) we have

$$\nu' = \nu \pm 3 \quad \text{or} \quad \nu' = \nu \pm 1. \quad (50.5a)$$

Let us consider as an example the case $\nu' = \nu + 3$, then the only possibility we may have in the number of intermediate quanta is

$$\nu_2 = \nu + 1, \nu_1 = \nu_2 + 1 = \nu + 2, \nu' = \nu_1 + 1 = \nu + 3, \quad (50.5b)$$

and for all terms in the summation over ν_1, ν_2 the phase will be -1 . For the case $\nu' = \nu - 3$, the analysis is the same and the phase is again (-1) . For the case when $\nu' = \nu \pm 1$, Hess *et al.* [20] have shown the convenience of symmetrizing the operator (49.3) with a factor $(1/3)$ in front, to find again that the effect of the phase terms just produces the factor $(1/3)$. Thus our conclusion is that

$$\langle\nu'|\{[\pi \times \alpha]^2 \times \pi\}^0|\nu\rangle = \langle\nu'|\{[\alpha \times \alpha]^2 \times \alpha\}^0|\nu\rangle C(\nu' - \nu), \quad (50.6)$$

where as $\nu' - \nu = \pm 3$ or ± 1 , we obtain

$$C(\pm 3) = -1, \quad C(\pm 1) = (1/3). \quad (50.7)$$

As in turn we have that

$$\{[\alpha \times \alpha]^2 \times \alpha\}^0 = -\sqrt{\frac{2}{35}}\beta^3 \cos 3\gamma = -\sqrt{\frac{2}{35}}\beta^3 \phi_0^{310}(\gamma), \quad (50.8)$$

we see that the matrix elements of the term (49.3) of the kinetic energy reduce to one of the type discussed in (49.15).

For the last term of Eq. (49.2) for the kinetic energy, we first have to hermitize and symmetrize, which we indicate by the index s in the expression, and by a reasoning similar to the one given for the term (49.3) we get [20]

$$\begin{aligned} &\langle\nu'|\{[\pi \times \pi]^0 \times [\alpha \times \alpha]^0\}_s^0|\nu\rangle \\ &= (-1)^{\frac{\nu'-\nu}{2}} \langle\nu'|\{[\alpha \times \alpha]^0 \times [\alpha \times \alpha]^0\}_s^0|\nu\rangle C'(\nu' - \nu) \\ &= (-1)^{\frac{\nu'-\nu}{2}} (6/5) \langle\nu'|\kappa'\ell'L'M'|\beta^4|\nu\kappa\ell LM\rangle C'(\nu' - \nu), \end{aligned} \quad (50.9)$$

which again is of the form (49.15) and where from (43.19) the selection rules are $\nu' = \nu \pm 4, \nu' = \nu \pm 2, \nu' = \nu$. The coefficients $C'(\nu' - \nu)$ now take the values

$$C'(\pm 4) = -1, \quad C'(\pm 2) = 0, \quad C'(0) = (1/3). \quad (50.10)$$

Thus we have reduced all the kinetic energy terms $K(\alpha_m, \pi_m)$ that we considered in (49.2), to those whose evaluation we discussed in the previous section.

c) Application to energy levels and transition probabilities in ^{238}U

To determine the Hamiltonian of a nucleus we have to specify the coefficients B_3, B_4 in the extra terms of the kinetic energy (49.2) as well as $V_{\rho\ell}$

of the potential energy in (49.4). In the analysis of Hess *et al.* [20] the potential is given as a linear combination of terms of the form

$$\beta^{\rho'} \cos 3\gamma, \quad (50.11)$$

where ρ' is any integer. This implies that some terms of the potential are not *polynomials* in the α_m . Their calculation though can still be done using Eq. (49.15), because it is valid not only for ρ integer, but also when it is half-integer or negative, as may happen because ρ' and ρ are related by

$$\rho' = 2\rho + 3\ell. \quad (50.12)$$

The analysis of Hess *et al.* [20] then gives us the values $B_3, B_4, V_{\rho\ell}$ (in the latter case, for several ρ 's and ℓ 's) by adjusting them by a mean square fit to the energy levels of a nuclei which, in the case we will discuss here, will be ^{238}U . Note though that Hess *et al.* [20] have B_2 and C_2 also as parameters while here we use units where $\hbar = B_2 = C_2 = 1$. It is easy though to translate their results to our units in which $B_3, B_4, V_{\rho\ell}$ are dimensionless, and we get then the values

$$B_3 = 0.0392372, \quad (50.13a)$$

$$B_4 = 0, \quad (50.13b)$$

while the $V_{\rho\ell}$ appear in the following Table IX.1.

With this definite Hamiltonian \mathcal{H} we can calculate its matrix elements:

$$\langle \nu' \kappa' \ell' L' M' | \mathcal{H} | \nu \kappa \ell L M \rangle, \quad (50.14)$$

where of course the L is fixed as it is an integral of motion. The values of ν, ν' are taken from 0 to 30 quanta with the corresponding numbers for κ, ℓ and κ', ℓ' that are compatible with the chosen L .

The diagonalization of the matrix whose elements are (50.14), then provides us with the energy levels associated with a given L , as well as the corresponding eigenstates. The latter can in turn be used to calculate the quadrupole transition probabilities of (49.13) from the state with a given L to one with $L + 2$. For this purpose it is convenient to note the selection rules for the two parts of Q_m , i.e., α_m and $[\alpha \times \alpha]_m^2$, which are given below, with Δ indicating the change in the corresponding quantum number:

$$\begin{array}{ccc|c} & \Delta\nu & \Delta\kappa & |\Delta L| \\ \alpha_m & \pm 1 & \pm 1 & \leq 2 \\ [\alpha \times \alpha]_m^2 & 0, \pm 2 & 0, \pm 2 & \leq 2 \end{array} \quad (50.15)$$

Table IX.1. Coefficients $V_{\rho\ell}$ defined in Eq. (49.4) in which $2\rho + 3\ell$ and ℓ are always non-negative integers, but ρ is not restricted.

$2\rho + 3\ell$	ρ	ℓ	$V_{\rho\ell}$
2	1	0	-1.39694
3	3/2	0	-1.16499 · 10 ⁻³
4	2	0	+0.04579
5	5/2	0	+2.87456 · 10 ⁻⁶
6	3	0	+2.80314 · 10 ⁻⁴
2	-1/2	1	-0.108120
3	0	1	-0.08881
5	1	1	+9.37409 · 10 ⁻⁵
2	-2	2	+0.10996
3	-3/2	2	+5.98211 · 10 ⁻³
6	0	2	-4.74705 · 10 ⁻⁴
2	-7/2	3	+6.64500 · 10 ⁻³
3	-3	3	+5.62924 · 10 ⁻⁴
2	-5	4	+0.01864
3	-9/2	4	+8.31749 · 10 ⁻⁴

It turns out that the lowest eigenvalues of the matrix for each L are connected by strong quadrupole transition $B(E2)$ and so they form a band which, in Table IX.2 appear first with the value of the orbital angular momentum L and an index 1. The second eigenvalues for each even L appear next in a band and have an index 2 for each L , while the third eigenvalues have an index 3 though there one has also contributions of the first eigenvalue for L odd. In Table IX.2 we return our results to standard units so the theoretical energies are given in MeV. Taking the ground state 0_1^+ at value 0, we give all the values of the other levels referred to this origin and the comparison with experiment (in parenthesis), when the latter is available. The agreement is quite good, as can be seen even better if one uses the rotation vibration model notation [8] and refers to the levels with indices 1,2,3 in Table IX.2 as the ground, β and γ bands [20] in Fig. IX.2. In particular for the ground band there are experimental results up to orbital angular momentum $L = 30$ and they agree very well with those predicted by the theory.

Table IX.2. Energies in the ground state and two side bands of ^{238}U as a function of the total angular momentum and parity of the states. Experimental values are given in parentheses.

State	Energy [MeV]	State	Energy [MeV]
0_1^+ (abs)	-3.190	26_1^+	3.938 (4.019)
2_1^+	0.046 (0.045)	28_1^+	4.452 (4.518)
4_1^+	0.150 (0.148)	30_1^+	4.988 (5.036)
6_1^+	0.307 (0.307)	32_1^+	5.544
8_1^+	0.512 (0.518)	34_1^+	6.118
10_1^+	0.761 (0.776)	0_2^+	0.970 (0.993)
12_1^+	1.050 (1.077)	2_2^+	1.033 (1.035)
14_1^+	1.374 (1.415)	4_2^+	1.154 (1.127)
16_1^+	1.731 (1.788)	6_2^+	1.326 (1.270)
18_1^+	2.119 (2.191)	2_3^+	1.067 (1.060)
20_1^+	2.535 (2.619)	3_3^+	1.121 (1.106)
22_1^+	2.978 (3.068)	4_3^+	1.212 (1.168)
24_1^+	3.447 (3.535)		

With the values of the parameter $V_{\rho\ell}$ given in Table IX.1 Hess *et al.* [20] calculate the potential energy surface of ^{238}U , shown also in Fig. IX.2, and they get a minimum at $\gamma = 0$ so ^{238}U is a prolate nucleus. The form of the potential as function of β when $\gamma = 0^\circ$ and $\gamma = 60^\circ$ is also drawn in Fig. IX.2.

Finally in Table IX.3 we give [20] the quadrupole transition probabilities, *i.e.*, the $B(E2)$ in units of the electron charge squared e^2 by barns (10^{-24} cm^2) squared b^2 , which imply that the Q_m of (49.13) is multiplied by an appropriate factor, as indicated in the table caption.

The initial and final nuclear states are indicated by their angular momentum and the band (indices 1,2,3 or $1,\beta,\gamma$) to which they belong. The transition always involves a change $\Delta L = 2$ in the angular momentum. When available, experimental values are also given in parenthesis in Table IX.2, and the agreement is good.

51. EXTENSION OF ANALYSIS TO ODD ANGULAR MOMENTA

Table IX.3. $B(E2)$ -values within the ground state band of ^{238}U in $e^2 b^2$ units. The values of the static quadrupole momentum for the lowest 2^+ levels are given in eb units. Experimental values are given in parentheses. In this table, e stands for the charge of the proton and b for barns, *i.e.*, $b = 10^{-24} \text{ cm}^2$.

Transition		$B(E2)(e^2 b^2)$
0_1^+	\rightarrow	2_1^+
2_1^+	\rightarrow	4_1^+
4_1^+	\rightarrow	6_1^+
6_1^+	\rightarrow	8_1^+
8_1^+	\rightarrow	10_1^+
10_1^+	\rightarrow	12_1^+
12_1^+	\rightarrow	14_1^+
14_1^+	\rightarrow	16_1^+
16_1^+	\rightarrow	18_1^+
18_1^+	\rightarrow	20_1^+
20_1^+	\rightarrow	22_1^+
22_1^+	\rightarrow	24_1^+
24_1^+	\rightarrow	26_1^+
26_1^+	\rightarrow	28_1^+
28_1^+	\rightarrow	30_1^+
0_1^+	\rightarrow	$2_2^+ (2_\beta^+)$
0_1^+	\rightarrow	$2_3^+ (2_\gamma^+)$

We see then that quadrupole collective motions in nuclei can be described quite effectively with the help of the five-dimensional oscillator, as it was developed in this chapter. In particular, the computer programs for these types of calculations [19,23,24] make them now very feasible and quick and we would like to point out the discussion of Hess *et al.* [25] for W, Pt, Os isotopes as examples of this type of applications.

51 Extension of the Analysis to Odd Angular Momenta

As indicated at the end of Section 46, the discussion in the previous pages was restricted to even orbital angular momenta L , particularly as in the application to the nucleus ^{238}U these are the more relevant ones. We now proceed to extend our results to odd L , to have a complete formalism for dealing with quadrupole collective vibrations in nuclei.

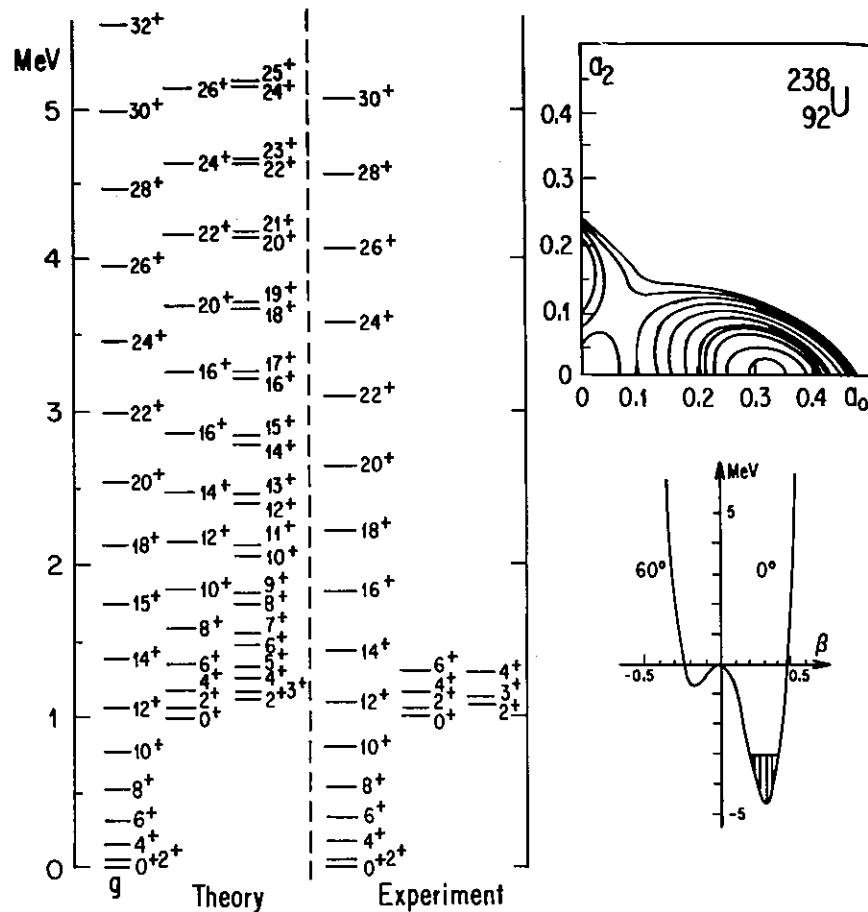


Figure IX.2. Theoretical energy spectrum of ^{238}U compared with experiment. On the right hand side the Potential Energy Surface and a cut through $\gamma = 0^\circ$ and 60° are given (P. O. Hess *et al.*, reference [20]).

It is convenient to designate in this section with a bar above, the magnitude being discussed when it refers to odd angular momentum. Thus when we write L we mean even and \bar{L} odd values of the angular momenta. We designate also by κ the one appearing as eigenvalue $\kappa(\kappa + 3)$ of the \mathcal{L}^2 of (44.6), *i.e.*, the seniority when the orbital angular momentum is even, *i.e.*, given by L . The corresponding one for \bar{L} will be called $\bar{\kappa}$.

The analysis leading to the ket $|\kappa\ell L\rangle$ of (46.17) suggests that the particle-hole states for \bar{L} could be written as

$$|\bar{\kappa}\ell\bar{L}\rangle = (\hat{a}_2^+)^{\sigma} \xi_2^{\tau} [3, 3][3, 0]^{\ell+\tau}|0\rangle, \quad (51.1)$$

where \hat{a}_m^+ , $m = 2, 1, 0, -1, -2$, is given by (46.7), $[3, 0]$ by (45.20), when we replace η_m by \hat{a}_m^+ , and $[3, 3]$ by (45.10b), again replacing η_m by \hat{a}_m^+ , but which we write explicitly as

$$[3, 3] = 2\hat{a}_{-1}^+(\hat{a}_2^+)^2 - \sqrt{6}\hat{a}_2^+\hat{a}_1^+\hat{a}_0^+ + (\hat{a}_1^+)^3. \quad (51.2)$$

The values of $\bar{\kappa}$, \bar{L} will now be related with σ, τ by

$$\bar{L} = 2(\sigma + \tau) + 3, \quad (51.3a)$$

$$\bar{\kappa} = \sigma + 2\tau + 3\ell + 3. \quad (51.3b)$$

As in the discussion for $|\kappa\ell L\rangle$ in section 47 we have to express the state in Eq. (51.1), purely in terms of the creation operators η_m and, after achieving this, it can be immediately written in terms of the epd's of $\alpha'_m s$ by using Dragt's theorem. The final form of the $|\bar{\kappa}\ell\bar{L}\rangle$ in terms of the variables $\vartheta_1, \vartheta_2, \vartheta_3, \beta, \gamma$, can then be obtained by a procedure similar to the one carried out in section 48.

To implement the program of the previous paragraph we start by expressing the $|\bar{\kappa}\ell\bar{L}\rangle$ of (51.1) in the form

$$|\bar{\kappa}\ell\bar{L}\rangle = (\hat{a}_2^+)^{\sigma} \xi_2^{\tau} |3\ell + 3\tau + 3, \ell + \tau, 3\rangle, \quad (51.4)$$

where the last ket can be expanded in terms of the epd in the form

$$\begin{aligned} |3\ell + 3, \ell, 3\rangle &= [3, 3][3, 0]^{\ell}|0\rangle \\ &= (3, 3) \sum_r \bar{B}_r^{\ell} (2, 0)^{3\tau} (3, 0)^{\ell-2\tau}|0\rangle, \end{aligned} \quad (51.5)$$

with (ν, L) given by (45.10a,b) and (45.20).

To determine the coefficients \bar{B}_r^{ℓ} we recall that the state $|3\ell + 3, \ell, 3\rangle$ has actually been determined directly in (44.40) in terms of the $\vartheta_1, \vartheta_2, \vartheta_3, \beta, \gamma$ and thus we can write

$$\begin{aligned}
|3\ell+3, \ell, 3\rangle &= \beta^{3\ell+3} P_{\ell+1}^1(x) \left[D_{32}^{3*}(\vartheta_i) - D_{3-2}^{3*}(\vartheta_i) \right] \exp(-\beta^2/2) \\
&= -\beta^{3\ell+3} (1-x^2)^{1/2} \left[D_{32}^{3*}(\vartheta_i) - D_{3-2}^{3*}(\vartheta_i) \right] \exp(-\beta^2/2) \\
&\quad \times \sum_r \left[(-1)^r \frac{(2\ell+1-2r)!!}{(\ell-2r)!(2r)!!} x^{\ell-2r} \right] \\
&= \left\{ \beta^{3\ell+3} \sin 3\gamma \left[D_{32}^{3*}(\vartheta_i) - D_{3-2}^{3*}(\vartheta_i) \right] \right\} (-1)^{\ell+1} 2^{-\ell/2} \\
&\quad \times \exp(-\beta^2/2) \sum_r \left[\frac{(-1)^r (2\ell+1-2r)!!}{(\ell-2r)!(r)!} \right] \{2, 0\}^{3r} \{3, 0\}^{\ell-2r}, \quad (51.6)
\end{aligned}$$

where we made use of the expansion in x of the associated Legendre polynomial $P_{\ell+1}^1(x)$, where $x = \cos 3\gamma$, and of the relations

$$\{2, 0\} = \beta^2, \quad (51.7a)$$

$$\{3, 0\} = -\sqrt{2}\beta^3 \cos 3\gamma = -\sqrt{2}\beta^3 x, \quad (51.7b)$$

which follow from (44.10a) and (44.20).

From Dragt's theorem that relates epd's $\{\nu, L\}$ in the α'_m 's with (ν, L) in η_m for harmonic states, as discussed in section 47, we see from (51.6), where the first curly bracket can be identified with $\{3, 3\}$, that \bar{B}_r^ℓ in (51.5) can take the form

$$\bar{B}_r^\ell = \frac{(-1)^r (2\ell+1-2r)!!}{(\ell-2r)! r!}. \quad (51.8)$$

The application now of $(a_2^+)^{\sigma} \xi_2^{\tau}$ to the state $|3\ell+3\tau+3, \ell+\tau, 3\rangle$ can be done exactly by the same procedure as in section 47, to obtain first a polynomial in the epd (ν, L) of η_m , and then to translate it to the epd $\{\nu, L\}$ in the α_m with the extra factor $\exp(-\beta^2/2)$. Thus using, in particular, the relation $[\xi_2, (3, 3)] = 0$, we get

$$\begin{aligned}
|\bar{\kappa}\ell\bar{L}\rangle &= \{3, 3\} P_{\kappa\ell L}(\alpha_m) \exp(-\beta^2/2) \\
&= \exp(-\beta^2/2) \{3, 3\} \sum_{r,n} \left[\bar{C}_{rn}^{\sigma\tau\ell} \{1, 2\}^{\sigma+\tau-n} \{2, 2\}^n \right. \\
&\quad \times \left. \{3, 0\}^{\ell+\tau-2r-n} \{2, 0\}^{3r-\tau+n} \right], \quad (51.9)
\end{aligned}$$

where $\kappa = \bar{\kappa} - 3$, $L = \bar{L} - 3$ and the coefficient $\bar{C}_{rn}^{\sigma\tau\ell}$ becomes

$$\begin{aligned}
\bar{C}_{rn}^{\sigma\tau\ell} &= \bar{B}_r^{\ell+\tau} 2^{\tau-n} 3^n \frac{(\ell+\tau-2r)!(3r)!}{(\ell+\tau-2r-n)!} \\
&\quad \times \sum_s \left[\binom{\tau+s}{n} 2^s \frac{R_s^\sigma(3\ell+2\tau+3-s)}{(3r-\tau+n-s)!} \right] \\
&= \frac{3^n \sigma!(\kappa+3)!(-1)^r 2^r (2\ell+2\tau+1-2r)!(3r)!}{2^{\ell+n} n! (2\kappa+7)! r! (\ell+\tau-r)! (\ell+\tau-n-2r)!} \\
&\quad \times \sum_s \left[\frac{(-4)^s (\tau+s)! (2\kappa+7-2s)!}{s! (\sigma-s)! (\tau-n+s)! (3r-\tau+n-s)! (\kappa+3-s)!} \right]. \quad (51.10)
\end{aligned}$$

We have been able, for odd \bar{L} , to write the state $|\bar{\kappa}\ell\bar{L}\rangle$ in terms of a polynomial expression in terms of the epd $\{\nu, L\}$ of the α_m . We want though to express it in terms of the variables $\vartheta_1, \vartheta_2, \vartheta_3, \beta, \gamma$ as was done in section 48 for even L . This implies writing

$$\{3, 3\} P_{\kappa\ell L}(\alpha_m) = \beta^{\bar{\kappa}} \sum_{\bar{K}} \phi_{\bar{K}}^{\bar{\kappa}\ell\bar{L}}(\gamma) D_{\bar{L}\bar{K}}^{\bar{L}}(\vartheta_i), \quad (51.11)$$

and thus from the discussion section 48 we have that

$$\phi_{\bar{K}}^{\bar{\kappa}\ell\bar{L}}(\gamma) = \sum_n G_{\bar{K}}^{n\bar{L}}(\gamma) \bar{f}_n^{\sigma\tau\ell}(x), \quad (51.12)$$

where

$$\bar{f}_n^{\sigma\tau\ell}(x) = (-1)^{\ell+\tau-n} 2^{(\ell+\tau-n+\kappa)/2} \sum_r \bar{C}_{rn}^{\sigma\tau\ell} 2^{-r} x^{\ell+\tau-n-2r} \quad (51.13)$$

is, except for a constant factor, similar to $f_n^{\sigma\tau\ell}$ of (48.4) with C being replaced by \bar{C} and

$$\begin{aligned}
G_{\bar{K}}^{n\bar{L}}(\gamma) &= (-1)^{1+\bar{K}} \sqrt{2\bar{L}+1} \\
&\quad \times \sum_{K,k} \binom{L}{K} \binom{3}{k} \binom{\bar{L}}{-\bar{K}} G_K^{nL}(\gamma) g_k^{(3)}(\gamma). \quad (51.14)
\end{aligned}$$

In (51.12) we have, as before, $x = \cos 3\gamma$ while in (51.14) we have a $3j$ coefficient of $O(3)$, $G_K^{nL}(\gamma)$, with $L = \bar{L} - 3$, is given by (48.13) while $g_k^{(3)}(\gamma)$ comes from the $\{3, 3\}$ in (51.11) and, in terms of the a_m fixed in the body given by (43.27), it has the form

$$\begin{aligned}
g_k^{(3)}(\gamma) &= \sqrt{14/3} \beta^{-3} \{ [a \times a]^2 \times a \}_k^3 \\
&= \frac{1}{\sqrt{3}} \sin 3\gamma (\delta_{k,2} - \delta_{k,-2}). \quad (51.15)
\end{aligned}$$

From (51.15) and the properties of the $3j$ coefficients, we conclude that

$$G_{\bar{K}}^{nL}(\gamma) = -G_{-\bar{K}}^{n\bar{L}}(\gamma), \quad (51.16)$$

and thus the symmetry properties of the $\phi_{\bar{K}}^{n\bar{L}}(\gamma)$ given in (48.16), are changed to the form

$$\phi_{\bar{K}}^{\bar{n}\bar{L}}(\gamma) = -\phi_{-\bar{K}}^{\bar{n}\bar{L}}(\gamma), \quad (51.17)$$

as was required from our initial analysis in (44.28).

By the same procedure as discussed in section 48, we can pass from the state $|\bar{k}\ell\bar{L}\rangle$ to the complete ket

$$|\bar{\nu}\bar{k}\ell\bar{L}\bar{M}\rangle, \quad (51.18)$$

and thus all of the results derived in section 49 are valid both for L even and \bar{L} odd.

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Chapter X

The Six-Dimensional Oscillator and the Interacting Boson Model

As mentioned in the previous chapter, there are many models for the description of collective structure in nuclei. One of the most successful is the Interacting Boson Model (IBM) proposed originally by Arima and Iachello [1], and continued later by many authors. A good compendium of the work done in this field in the past 20 years is given in Part III of a book of Frank and Van Isacker [2], in which the reader can also find extensive references to the literature on this subject.

Our interest in this field will be restricted to showing that its basic Hamiltonian is a six-dimensional oscillator. As the symmetry group of the latter is the unitary group U(6), we shall proceed to discuss the different chains of its subgroups ending in the O(3) associated with angular momentum, and find the relations between them.

Once we attain the objective indicated in the previous paragraph, we shall proceed to show that the most general Hamiltonian that one can form of one- and two-body interactions, can be expressed in terms of the Casimir operators of the chains of groups mentioned, and thus a mathematical procedure is established both for pure (*i.e.*, associated with a single chain) and mixed systems of states. Applications to specific nuclei will be given at the end of the chapter.

We first review briefly the origin of the IBM.

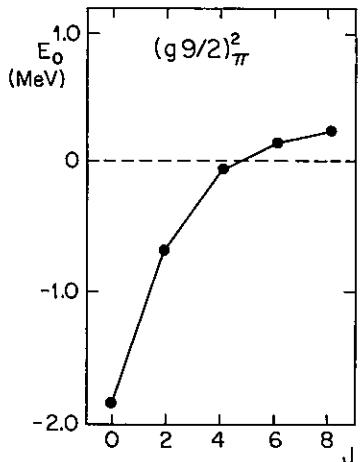


Figure X.1. Matrix elements for the two proton configuration in the $g_{9/2}$ shell. One gets strong negative values, and thus strong attraction, for total angular momentum $J = 0, 2$, while for larger J 's the values are zero or positive indicating a repulsion. (Taken from O. Scholten, Ph.D. Thesis, Groningen, 1980).

52 The Interacting Boson Model

As was mentioned in several of the previous Chapters the shell model [3] has provided an extremely powerful tool for our understanding of nuclear structure. Nevertheless if we take the model seriously for a nucleus such as ^{156}Sm , we find out that we need to start with 10^{14} states. Obviously a truncation is necessary if we hope to get meaningful results for our calculations.

A suggestion in this direction is given by the fact that, for two nucleon states in a given shell, we get matrix elements that are strongly negative and thus strongly attractive for angular momentum $J = 0$ and they still remain negative and attractive for $J = 2$. For higher J they become positive and thus repulsive as indicated in Fig. X.1 for $(g_{9/2})^2$.

It is therefore suggestive to consider specific two particle states in many shell configurations of angular momentum $J = 0, 2$ which we designate by the kets

$$|S\rangle = \sum_j a_j |[j \times j]^0\rangle, \quad (52.1a)$$

$$|D\rangle = \sum_{jj'} b_{jj'} |[j \times j']^2\rangle, \quad (52.1b)$$

and to construct from them a general state for $2N$ valence nucleons as

$$|S^{N-\nu} D^\nu, L\rangle, \quad (52.2)$$

where in (52.2) we designate by ν the number of D pairs of the type (52.1b) coupled to a total angular momentum L .

If we work with states of type (52.2) only, with certain restrictions on the seniority of the D pairs, the number of states is drastically reduced from 10^{14} to 10^3 or, on occasions, even a much smaller number.

So far we have been speaking of fermion pair coupled to angular momentum 0 or 2. It proved extremely useful [1] to replace these pair of fermions by bosons associated with the angular momenta 2 and 0. For the former we can use the notation in terms of the creation operators η_m , $m = 2, 1, 0, -1, -2$ given in (43.19). For the latter our notation requires a single scalar creation operator which we shall denote $\bar{\eta}$. We can thus establish the correspondence

$$|S^{N-\nu} D^\nu, L\rangle \rightarrow \bar{\eta}^{N-\nu} \left[(\eta_m)^\nu \right]^L |0\rangle, \quad (52.3)$$

where $|0\rangle$ designates the boson vacuum and the ν operators η_m are coupled to total angular momentum L .

If we are in this boson picture it is a question of considering six creation, and their corresponding annihilation, operators

$$\eta_m, \quad m = 2, 1, 0, -1, -2; \quad \bar{\eta}, \quad (52.4)$$

$$\xi^m, \quad m = 2, 1, 0, -1, -2; \quad \bar{\xi}, \quad (52.5)$$

that have the commutation rules

$$[\eta_m, \eta_{m'}] = 0, [\xi^m, \xi^{m'}] = 0, [\xi^{m'}, \eta_m] = \delta_m^{m'}, \quad (52.6a)$$

$$[\eta_m, \bar{\eta}] = [\eta_m, \bar{\xi}] = [\xi_m, \bar{\eta}] = [\xi^m, \bar{\xi}] = 0, \quad (52.6b)$$

$$[\bar{\xi}, \bar{\eta}] = 1. \quad (52.6c)$$

The group associated with products of the operators (52.4,5) is, from the discussion of Chapter VII, clearly given by the unitary one in six-dimension $U(6)$ whose 36 generators are

$$\eta_m \xi^{m'}, \eta_m \bar{\xi}, \bar{\eta} \xi^{m'}, \bar{\eta} \bar{\xi}; \quad m, m' = 2, 1, 0, -1, -2, \quad (52.7)$$

and its first order Casimir operator is

$$\hat{N} = \sum_{m=-2}^2 \eta_m \xi^m + \bar{\eta} \bar{\xi}. \quad (52.8)$$

Comparing it with Eq. (43.20) we see that, except for an additive numerical term, this is the Hamiltonian of a six-dimensional harmonic oscillator.

Before discussing more general Hamiltonians that we can form from the generators (52.7) of the $U(6)$ group, and applying them to states of the form (52.3) to get spectra comparable with experiment, we proceed to analyze the mathematical structure of the problem.

53 Chains of Groups Associated with the Six-Dimensional Oscillator

As mentioned in the previous section the symmetry group of our oscillator has as its components 6×6 unitary matrices which we designate by $U(6)$. The subgroup $O(3)$ is also a 6×6 matrix of the form

$$O(3) = \begin{bmatrix} \|D_{mk}^2(\vartheta_1, \vartheta_2, \vartheta_3)\| & 0 \\ 0 & 1 \end{bmatrix}, \quad (53.1)$$

and as $m, k = 2, 1, 0, -1, -2$, the 5×5 unitary matrix appearing there is the same as the one in (46.1), corresponding to the representation $L = 2$ of the $O(3)$ group.

We now proceed to indicate three possible chains of groups that start with $U(6)$ and end with $O(3)$, and give their corresponding generators and Casimir operators.

a) The chain $U(6) \supset U(5) \supset O(5) \supset O(3)$

Looking at the creation operators (52.4), that could be considered as a six-dimensional complex vector on which the $U(6)$ matrix acts, we see that a possible chain of groups is

$$\begin{aligned} & U(6) \\ & \cup \\ & \left(\begin{array}{cc} U(5) & 0 \\ 0 & 1 \end{array} \right) \\ & \cup \\ & \left(\begin{array}{cc} O(5) & 0 \\ 0 & 1 \end{array} \right) \\ & \cup \\ & O(3) \end{aligned} \quad (53.2)$$

The subgroups are clearly those we discussed in the previous chapter where we dealt with the five-dimensional oscillator. Thus from (46.1,2) the generators of the subgroups indicated are

$$U(5); C_m^{m'} = \eta_m \xi^{m'}; \quad m, m' = 2, 1, 0, -1, -2, \quad (53.3a)$$

$$O(5); L_{mm'} = (1/\sqrt{2})(C_{mm'} - C_{m'm}), \quad (53.3b)$$

$$O(3); \hat{L}_q = (-1)^q \sqrt{15} \sum_{m,m'} \begin{pmatrix} 2 & 2 & 1 \\ m & m' & -q \end{pmatrix} L_{m,m'}, \quad (53.3c)$$

where for (53.3c) we used (45.6) and properties of the $3j$ coefficients, as well as the definition (53.3b) of $L_{m,m'}$.

As we will be dealing with the symmetric, *i.e.*, one row irreps of $U(6)$, we need only the corresponding ones for $U(5)$ and thus the required Casimir operator of the latter is

$$\hat{N} = \sum_{m=-2}^2 C_m^m, \quad (53.4a)$$

while those of $O(5)$ and $O(3)$ will be respectively

$$L^2 = \sum_{m,m'} L_{mm'} L^{m'm}, \quad (53.4b)$$

$$\hat{L}^2 = \sum_{q=-1}^1 \hat{L}_q \hat{L}^q = \sum_{q=-1}^1 (-1)^q \hat{L}_q \hat{L}_{-q}. \quad (53.4c)$$

In the previous section we indicated that the eigenvalues of the Casimir operators in (53.4) are

$$\nu, \quad \kappa(\kappa + 3), \quad L(L + 1). \quad (53.5)$$

If we denote by N the eigenvalue of the operator \hat{N} of $U(6)$ in (52.8), then clearly the states for the chain (53.2) could be denoted by

$$|N\nu\kappa\ell LM\rangle = |\nu\kappa\ell LM\rangle \left\{ [(N - \nu)!]^{-\frac{1}{2}} \bar{\eta}^{N-\nu} |0\rangle \right\}, \quad (53.6)$$

where the first ket was discussed extensively in the previous chapter, while the curly bracket indicates the state corresponding to $N - \nu$ s bosons.

The basis (53.6) will be the one we shall normally use in our discussion of IBM when matrix elements are required, as it has an explicit expression in terms of creation operators, as well as in coordinates α_m , $m = 2, 1, 0, -1, -2$ or $\beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3$. In the latter cases we would have to add a coordinate $\bar{\alpha}$ associated with $\bar{\eta}$, but this is trivial as the curly bracket in (53.6) corresponds to the wave function of a one-dimensional oscillator.

b) The chain $U(6) \supset O(6) \supset O(5) \supset O(3)$

As in section 46, where we introduced an $O(5)$ subgroup of $U(5)$, we can now have an $O(6)$ subgroup of $U(6)$, that would imply that in the chain (53.2) we replace the term containing $U(5)$ by a 6×6 orthogonal matrix in complex form $O(6)$.

The only new generators that we require are now those of $O(6)$ and for this purpose it is convenient to use for creation an annihilation operators the notation $\eta_{\ell m}, \xi_{\ell m}, \ell = 0, 2$ given in terms of (52.4,5) by

$$\eta_{2m} = \eta_m, \xi^{2m} = \xi^m, \eta_{oo} = \bar{\eta}, \xi^{oo} = \bar{\xi}. \quad (53.7)$$

The generators of $U(6)$ can then also be written as

$$C_{\ell m}^{\ell' m'} = \eta_{\ell m} \xi^{\ell' m'}, \ell, \ell' = 0, 2, \quad (53.8)$$

and thus the ones of $O(6)$ become

$$\mathbb{L}_{\ell m, \ell' m'} = \frac{1}{\sqrt{2}} (C_{\ell m, \ell' m'} - C_{\ell' m', \ell m}). \quad (53.9)$$

The Casimir operator of $O(6)$ is

$$\mathbb{L}^2 = \sum_{\ell, \ell'} \sum_{m, m'} \mathbb{L}_{\ell m, \ell' m'} \mathbb{L}^{\ell' m', \ell m} = \mathcal{L}^2 + \mathcal{K}^2, \quad (53.10)$$

where \mathcal{K}^2 , when we return to the notation (52.4,5), takes the form

53. CHAINS OF GROUPS ASSOCIATED

$$\begin{aligned} \mathcal{K}^2 &= \hat{N}(\bar{\eta}\bar{\xi} + 1) + (\hat{N} + 5)\bar{\eta}\bar{\xi} \\ &\quad - \left(\sum_m \eta_m \eta^m \right) \bar{\xi}^2 - \left(\sum_m \xi_m \xi^m \right) \bar{\eta}^2, \end{aligned} \quad (53.11)$$

with \hat{N} , being the number operator for the five-dimensional oscillator given by (45.5), and \mathcal{L}^2 is given by (46.4).

As $U(6)$ has only the single row representation characterized by N , the irreps of $O(6)$ will also be denoted by a single integer we write as ϱ , so the Casimir operator (53.10) of $O(6)$ takes the value [4]

$$\varrho(\varrho + 4). \quad (53.12)$$

The eigenstates for the chain of groups $U(6) \supset O(6) \supset O(5) \supset O(3)$ could be denoted as

$$|N\varrho\kappa\ell LM\rangle, \quad (53.13)$$

where we use a round ket rather than an angular one to distinguish them from the ket (53.6) of the previous chain. Note that, as in (44.29), we have the relation

$$\varrho = N, N - 2, N - 4, \dots, 1 \text{ or } 0. \quad (53.14)$$

In the following section we shall express the ket (53.13) as a linear combination of those of (53.6), and as both chains have $O(5) \supset O(3)$ in common, the transformation brackets required will not depend on ℓ, L, M so we could write them as

$$\langle N\nu\kappa | N\varrho\kappa \rangle. \quad (53.15)$$

These brackets would allow us to calculate the matrix elements of \mathbb{L}^2 , the Casimir operator of $O(6)$, in the chain $U(6) \supset U(5) \supset O(5) \supset O(3)$.

c) The chain $U(6) \supset U(3) \supset O(3)$

As discussed in Chapter VII, the irreducible representations of the $U(3)$ group can be characterized by (λ, μ, ρ) as indicated in Eq. (39.25). In particular, when they take the values $(2, 0, 0)$ the representation is six-dimensional and could be denoted by the 6×6 matrix

$$\mathcal{D}^{(2)}[U(3)], \quad (53.16)$$

where we suppressed the zeros in the upper index 2. We could then consider the chain

$$U(6) \supset D^{(2)}[U(3)] \supset \begin{bmatrix} \|D_{mk}^2(\vartheta_1, \vartheta_2, \vartheta_3)\| & 0 \\ 0 & 1 \end{bmatrix}, \quad (53.17)$$

as corresponding to the title of this subsection.

The states that are basis of the irreducible representations (BIR) (2,0,0) of $U(3)$, are clearly the three-dimensional harmonic oscillator ones $|2\ell m\rangle$ given in (38.6), where ℓ, m can take only the values $\ell = 0, m = 0; \ell = 2, m = 2, 1, 0, -1, -2$.

The nine generators of the $U(3)$ group were originally [5] the $\Gamma_1; L_q$, $q = 1, 0, -1; Q_m, m = 2, 1, 0, -1, 2$, given respectively by (38.4,11,12), and we now have to express them in the BIR $|2\ell m\rangle$. We have already done this with N in (52.8) and \hat{L}_q in (53.3c). For Q_m , we see from the discussion relating (39.4) with (39.5), and the properties of $3j$ coefficients, that we could write it as

$$Q_m = -(8\pi/15)^{1/2} \sum_{\ell' m'} \sum_{\ell'' m''} \langle 2\ell' m' | r^2 Y_{2m}(\theta, \phi) | 2\ell'' m'' \rangle \eta_{\ell' m'} \xi^{\ell'' m''}, \quad (53.18)$$

where we use the notation (53.7) for the creation and annihilation operators.

With the help of the explicit value of the matrix element in (53.18) given in (2.8), and employing the notation (52.4,5) we finally get

$$Q_m = \sqrt{\frac{7}{3}} [\eta \times \xi]_m^2 + \sqrt{\frac{4}{3}} (\bar{\eta} \xi_m + \eta_m \bar{\xi}), \quad (53.19)$$

where the multiplication sign indicates coupling to total angular momentum 2, and η, ξ stand for vectors whose five components are η_m and ξ_m , $m = 2, 1, 0, -1, -2$.

In section 55 we shall calculate the matrix elements of the operator Q_m with respect to the states that are BIR of the chain $U(6) \supset U(5) \supset O(5) \supset O(3)$, and with the help of them the corresponding matrix elements of

$$Q^2 = \sum_{m=-2}^2 (-1)^m Q_m Q_{-m}. \quad (53.20)$$

We shall show in Section 56 that the most general interaction in the IBM of one- and two-body types, can be expressed as a combination of the operators

$$\hat{N}, \hat{N}, \mathbb{L}^2, \mathcal{L}^2, Q^2, L^2, \quad (53.21)$$

and thus, as we indicated above, its finite matrix in the basis associated with the chain (53.2), can be obtained explicitly.

54 Transformation Brackets Between States in the $O(6)$ and $U(5)$ Chains of Groups

In Eq. (48.17) we wrote down the states for the $U(5) \supset O(5) \supset O(3) \supset O(2)$ chain of groups as

$$|\nu \kappa \ell LM\rangle = F_j^\kappa(\beta) \chi_M^{\kappa \ell L}(\gamma, \vartheta_i), \quad (54.1a)$$

where

$$\chi_M^{\kappa \ell L}(\gamma, \vartheta_i) = \sum_K \phi_K^{\kappa \ell L}(\gamma) D_{MK}^{L^*}(\vartheta_i), \quad (54.1b)$$

and $F_j^\kappa(\beta)$ is given in Eq. (44.31) with $j = \frac{1}{2}(\nu - \kappa)$.

If we now wish to consider the BIR of the above chain of groups but starting with $U(6)$, we see from (53.6) that we only need to multiply the ket (54.1) by the wave function of the one-dimensional oscillator

$$u_n(\bar{\alpha}) = \left[2^{-\frac{n}{2}} (n!)^{-1/2} \pi^{-1/4} \right] H_n(\bar{\alpha}) \exp(-\bar{\alpha}^2/2), \quad (54.2)$$

where $H_n(\bar{\alpha})$ is the Hermite polynomial of $\bar{\alpha}$, and the total number of quanta N characterizing the irreducible representation of $U(6)$ is

$$N = \nu + n. \quad (54.3)$$

We thus have the explicit expression for the ket

$$|N \nu \kappa \ell LM\rangle. \quad (54.4)$$

We now turn our attention to the chain $U(6) \supset O(6) \supset O(5) \supset O(3) \supset O(2)$ and note that the Casimir operator of $U(6)$, i.e., \hat{N} is the same, and that of $O(6)$ is given by \mathbb{L}^2 of (53.10), which contains the \mathcal{L}^2 of $O(5)$ plus the term \mathcal{K}^2 of (53.11).

Recalling the definitions of η_m, ξ_m in terms of α_m, π_m given in (43.19), and using a similar one for $\bar{\eta}, \bar{\xi}$, i.e.,

$$\bar{\eta} = (1/\sqrt{2})(\bar{\alpha} - i\bar{\pi}), \quad \bar{\xi} = (1/\sqrt{2})(\bar{\alpha} + i\bar{\pi}), \quad (54.5)$$

we easily get from (53.10,11) that

$$\begin{aligned} \mathbb{L}^2 &= \mathcal{L}^2 - \beta^2 \frac{\partial^2}{\partial \bar{\alpha}^2} - \left(\frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} - \frac{1}{\beta^2} \mathcal{L}^2 \right) \bar{\alpha}^2 \\ &\quad + \left(\beta \frac{\partial}{\partial \beta} + 5 \right) \bar{\alpha} \frac{\partial}{\partial \bar{\alpha}} + \beta \frac{\partial}{\partial \beta} \left(\bar{\alpha} \frac{\partial}{\partial \bar{\alpha}} + 1 \right), \end{aligned} \quad (54.6)$$

where we used the fact that $\pi_m = -i\partial/\partial\alpha^m$, $\bar{\pi} = -i\partial/\partial\bar{\alpha}$ and

$$\beta^2 = \sum_m \alpha_m \alpha^m, \quad (54.7a)$$

$$\beta\partial/\partial\beta = i \sum_m \alpha_m \pi^m, \quad (54.7b)$$

$$\hat{N} = \frac{1}{2}(\beta^2 + \pi^2) - \frac{5}{2}, \quad (54.7c)$$

$$\pi^2 = \sum_m \pi_m \pi^m = -\left(\frac{1}{\beta^4} \frac{\partial}{\partial\beta} \beta^4 \frac{\partial}{\partial\beta} - \frac{\mathcal{L}^2}{\beta^2} \right). \quad (54.7d)$$

Instead of using the variables

$$\bar{\alpha}, \beta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3, \quad (54.8)$$

for our wave functions, we consider new ones denoted as

$$b, \delta, \gamma, \vartheta_1, \vartheta_2, \vartheta_3, \quad (54.9)$$

where

$$\bar{\alpha} = b \cos \delta, \quad \beta = b \sin \delta. \quad (54.10)$$

From (54.6,10) it is straightforward to rewrite \mathbb{L}^2 as

$$\mathbb{L}^2 = -\frac{\partial^2}{\partial\delta^2} - 4\cot\delta \frac{\partial}{\partial\delta} + \frac{1}{\sin^2\delta} \mathcal{L}^2. \quad (54.11)$$

Clearly the eigenstates for the chain $U(6) \supset O(6) \supset O(5) \supset O(3)$ can be written as

$$|N\varrho\kappa\ell LM\rangle = B_{N\varrho\kappa} f_J^\varrho(b) g_\kappa^\varrho(\delta) \chi_M^{\kappa\ell L}(\gamma, \vartheta_i), \quad (54.12)$$

where $\chi_M^{\kappa\ell L}(\gamma, \vartheta_i)$ is given by (54.1b), $B_{N\varrho\kappa}$ is a normalization coefficient, while $g_\kappa^\varrho(\delta)$ satisfies the equation

$$\left[-\frac{d^2}{d\delta^2} - 4\cot\delta \frac{d}{d\delta} + \frac{\kappa(\kappa+3)}{\sin^2\delta} \right] g_\kappa^\varrho(\delta) = \varrho(\varrho+4) g_\kappa^\varrho(\delta). \quad (54.13)$$

In turn $f_J^\varrho(b)$ is determined by the equation

$$\left\{ \frac{1}{2} \left[-\frac{1}{b^5} \frac{\partial}{\partial b} b^5 \frac{\partial}{\partial b} + \frac{\varrho(\varrho+4)}{b^2} + b^2 \right] - 3 \right\} f_J^\varrho(b) = N f_J^\varrho(b), \quad (54.14)$$

where $J = (N - \varrho)/2$.

From (54.13) we obtain

$$g_\kappa^\varrho(\delta) = (\sin\delta)^\kappa C_{\varrho-\kappa}^{\kappa+2}(\cos\delta), \quad (54.15)$$

where C is a Gegenbauer polynomial [6] of the indices indicated. In turn from (54.14) we obtain

$$f_J^\varrho(b) = b^\varrho L_J^{\varrho+2}(b^2) \exp(-b^2/2), \quad (54.16)$$

where L is a Laguerre polynomial [6].

The normalization coefficient $B_{N\varrho\kappa}$ appearing in (54.12) can be obtained from well known integrals involving Gegenbauer and Laguerre polynomials [6] and its explicit value is [7]

$$B_{N\varrho\kappa} = 2^{\kappa+2}(\kappa+1)! \left\{ \frac{(\varrho-\kappa)![(N-\varrho)/2]!(\varrho+2)}{\pi(\varrho+\kappa+3)![(N+\varrho)/2+2]!} \right\}^{\frac{1}{2}}. \quad (54.17)$$

Thus the transformation brackets between states characterized by the $O(6)$ or $U(5)$ chain of groups implies the development of [7]

$$B_{N\varrho\kappa} f_J^\varrho(b) g_\kappa^\varrho(\delta) \quad (54.18)$$

in terms of the states

$$F_J^\kappa(\beta) u_n(\bar{\alpha}), \quad (54.19)$$

given by (44.31) and (54.2), and where b, δ are related to $\beta, \bar{\alpha}$ by (54.10). Note that in (54.18) there is a term $\exp(-b^2/2) = \exp(-\beta^2/2) \exp(-\bar{\alpha}^2/2)$ that cancels with the corresponding term in (54.19). Furthermore the function $g_\kappa^\varrho(\delta)$ of (54.15) can be expressed as a polynomial in powers of $\sin\delta$ and $\cos\delta$, and taking into account its product with β^ϱ in (54.16), we see from (54.10) that in (54.18) there are powers of $\beta, \bar{\alpha}$ and $b^2 = (\beta^2 + \bar{\alpha}^2)$. Thus the development of (54.18) in terms of (54.19) can be carried out in a systematic fashion and the details are given in Appendix B of reference [7].

Rather than use the compact notation $\langle N\nu\kappa | N\varrho\kappa \rangle$ of (53.15) for this transformation bracket we replaced N in the bra by $n = N - \nu$ appearing in (54.19), and write

$$\begin{aligned} \langle n\nu\kappa | N\varrho\kappa \rangle &= (-1)^{(N-\varrho+\nu-\kappa)/2} \\ &\times \left\{ \frac{2^{\varrho-\kappa} (\varrho+1)!(\varrho+2)(\nu+\kappa+3)!n![(N+\varrho)/2]!}{2^{N-\varrho} [(N+\varrho)/2+2]!(\varrho-\kappa)!(\varrho+\kappa+3)[(\nu+\kappa)/2+1]![(\nu-\kappa)/2]!} \right\}^{\frac{1}{2}} \\ &\times \sum_s \frac{[(N-\varrho)/2+1]_s [(\kappa-\varrho)/2]_s [(\kappa-\varrho+1)/2]_s}{s! [(N-\varrho-\nu+\kappa)/2+s]! [(-\varrho-1)]_s}, \end{aligned} \quad (54.20)$$

where $(x)_s$ is the Pochammer symbol:

$$(x)_s = x(x+1)\dots(x+s-1). \quad (54.21)$$

With the help of the transformation bracket (54.20) we can calculate the matrix of \mathbb{L}^2 , which is diagonal with values $\varrho(\varrho+4)$ in the O(6) chain, in the BIR associated with the U(5) chain.

55 Matrix Elements of \mathcal{Q}_m and \mathcal{Q}^2 with Respect to the BIR of a U(5) Chain of Groups

The \mathcal{Q}_m operator is given in (53.19) and using the expression (43.19) of η_m, ξ_m in terms of α_m, π_m and (54.5) of $\bar{\eta}, \bar{\xi}$ in terms of $\bar{\alpha}, \bar{\pi}$, we can write it as

$$\mathcal{Q}_m = \sqrt{\frac{7}{12}} \left\{ [\alpha \times \alpha]_m^2 + [\pi \times \pi]_m^2 \right\} + \sqrt{\frac{4}{3}} (\alpha_m \bar{\alpha} + \pi_m \bar{\pi}). \quad (55.1)$$

We would like first to discuss the matrix element

$$\left\langle N \nu'' \kappa'' \ell'' L'' M'' | \mathcal{Q}_m | N \nu' \kappa' \ell' L' M' \right\rangle, \quad (55.2)$$

where N is not changed in bra and ket as \mathcal{Q}_m is function of the generators of U(6), and thus commutes with its Casimir operator \hat{N} of (52.8).

In the discussion (50.3) of the matrix element of π_m with respect to the BIR in the chain $U(5) \supset O(5) \supset O(3)$, we showed that it is the same as that of α_m with the phase factor

$$(-1)^{\frac{\nu'' - \nu'}{2}}. \quad (55.3)$$

Repeating the argument with a full set of intermediate states, we see that the matrix element of $[\pi \times \pi]_m^2$ is equal to that of $[\alpha \times \alpha]_m^2$ multiplied by the same phase factor (55.3).

Turning now our attention to the operator $\pi_m \bar{\pi}$ we note, that for a one-dimensional oscillator whose ket we denote by $|n\rangle$ we also have

$$\langle n'' | \bar{\pi} | n' \rangle = (-1)^{\frac{n'' - n'}{2}} \langle n'' | \bar{\alpha} | n' \rangle, \quad (55.4)$$

as can be immediately seen if we write $\bar{\alpha}, \bar{\pi}$ in terms of $\bar{\eta}, \bar{\xi}$ using (54.5). As the product of phases

$$(-1)^{\frac{\nu'' - \nu'}{2}} (-1)^{\frac{n'' - n'}{2}} = 1, \quad (55.5)$$

55. MATRIX ELEMENTS OF \mathcal{Q}_m AND \mathcal{Q}^2

because $\nu'' + n'' = \nu' + n' = N$ we see that the matrix element of $\pi_m \bar{\pi}$ reduces to that of $\alpha_m \bar{\alpha}$.

In the matrix element (55.2) we shall replace the N in the ket by n' and in the bra by n'' , which are related with N and ν', ν'' as in the previous paragraph. Thus the matrix element (54.2) becomes

$$\begin{aligned} & \langle n'' \nu'' \kappa'' \ell'' L'' M'' | \sqrt{\frac{7}{12}} [1 + (-1)^{\frac{\nu'' - \nu'}{2}}] [\alpha \times \alpha]_m^2 \\ & \quad + \sqrt{\frac{16}{3}} \alpha_m \bar{\alpha} | n' \nu' \kappa' \ell' L' M' \rangle \\ & = \sqrt{\frac{1}{12}} \delta_{n'', n'} [1 + (-1)^{\frac{\nu'' - \nu'}{2}}] \langle \nu'' \kappa'' \ell'' L'' M'' | \beta^2 \\ & \quad \times \sum_K \phi_K^{202}(\gamma) D_{MK}^{2*}(\vartheta_i) |\nu' \kappa' \ell' L' M' \rangle \\ & + \sqrt{\frac{8}{3}} \left[\sqrt{n' + 1} \delta_{n'', n'+1} + \sqrt{n'} \delta_{n'', n'-1} \right] \langle \nu'' \kappa'' \ell'' L'' M'' | \beta \\ & \quad \times \sum_K \phi_K^{102} D_{MK}^{2*}(\vartheta_i) |\nu' \kappa' \ell' L' M' \rangle, \end{aligned} \quad (55.6)$$

where for the right hand side we used the expression for α_m and $[\alpha \times \alpha]_m^2$ given in (49.10) and (49.14) in terms of $\beta, \gamma, \vartheta_1, \vartheta_2$ and ϑ_3 .

The remaining matrix elements in (55.6) are exactly of the type (49.15) if we take $\varrho = 0, \kappa = 2$ or $1, \ell = 0$ and $L = 2$, and thus they can be evaluated by the procedure indicated at the end of section 49. Note that as $\nu'' = N - n'', \nu' = N - n'$ in the first matrix element in (55.6) we must take $\nu'' = \nu'$ while in the second $\nu'' = \nu' - 1$ or $\nu'' = \nu' + 1$ if we combine them with $\delta_{n'', n'+1}$ or $\delta_{n'', n'-1}$ respectively.

We recall that the ket $|\nu \kappa \ell LM\rangle$ is not orthonormal in the index ℓ , so before proceeding to try to obtain the matrix elements of \mathcal{Q}^2 from those of (55.6) we must indicate how to orthonormalize this BIR. For this purpose we note from (46.18) that the index ℓ satisfies the inequalities

$$\kappa - L \leq 3\ell \leq \kappa - (L/2) \text{ if } L \text{ is even} \quad (55.7a)$$

$$\kappa - L \leq 3\ell \leq \kappa - \frac{1}{2}(L+3) \text{ if } L \text{ is odd.} \quad (55.7b)$$

For fixed κ, L the relations (46.18) indicate that if there are values of ℓ that satisfy them, they will take all integer values between a minimum one ℓ_0 and a maximum $\bar{\ell}_0$. We define an index s as

$$s = \ell - \ell_0 + 1, \quad (55.8)$$

which takes the values

$$s = 1, 2, \dots, d(\kappa, L), \quad (55.9)$$

where $d(\kappa, L) = \bar{\ell}_0 - \ell_0 + 1$. Instead of the index ℓ in the ket (48.17) we could use the index s that takes the values (55.9), and thus write the ket for the full group chain (53.2) as

$$|n\nu\kappa sLM\rangle, \quad (55.10)$$

where, as before, $n + \nu = N$.

We already mentioned computer programs [8,9] that transform this set into an orthonormal one which we designate by the curly ket

$$|\mathcal{n}\nu\kappa tLM\rangle, \quad (55.11)$$

where t takes the values in the same range (55.9), and the ket (55.11) is a linear combination, with respect to the index s , of the kets (55.10).

As the kets (55.11) form a complete orthonormal set, we could write the matrix element of \mathcal{Q}^2 as

$$\begin{aligned} & \langle n''\nu''\kappa''t''L''M'' | \mathcal{Q}^2 | n'\nu'\kappa't'L'M' \rangle \\ &= \sum_{n\nu\kappa tLM} \sum_{m=-2}^2 [(-1)^m \langle n''\nu''\kappa''t''L''M'' | \mathcal{Q}_m | n\nu\kappa tLM \rangle \\ & \quad \times \langle n\nu\kappa tLM | \mathcal{Q}_{-m} | n'\nu'\kappa't'L'M' \rangle], \end{aligned} \quad (55.12)$$

where the matrix elements on the right hand side can be given in terms of linear combinations of those in (55.6). The strong selection rules after (55.6) make the summation finite and with a small number of terms.

We have thus achieved our purpose of expressing the \mathcal{Q}^2 , (which combined linearly with \hat{L}^2 and \hat{N}, \hat{N}^2 , as in (39.6), gives the second order Casimir operator of U(3)) in the BIR (53.2).

We shall proceed now to show that we have obtained all the elements required to get the matrix of the most general Hamiltonian in the IBM with one- and two-body terms.

56 The General Hamiltonian of the Interacting Boson Model

The most general two-body interaction involving d and s bosons can be expressed in the form [5]

$$\begin{aligned} V &= \frac{1}{2} \sum_{l_1 m_1, l_2 m_2} \sum_{l'_1 m'_1, l'_2 m'_2} \\ & \quad \times \left\{ \langle 2l_1 m_1, 2l_2 m_2 | V_{12} | 2l'_1 m'_1, 2l'_2 m'_2 \rangle \eta_{l_1 m_1} \eta_{l_2 m_2} \xi^{l'_1 m'_1} \xi^{l'_2 m'_2} \right\} \\ &= \frac{1}{2} \sum_{l_1, l_2} \sum_{l'_1, l'_2} \sum_L \left\{ \langle 2l_1, 2l_2, L | V_{12} | 2l'_1, 2l'_2, L \rangle \right. \\ & \quad \times \left. (-1)^{l'_1 + l'_2} (2L + 1)^{\frac{1}{2}} \left[[\eta_{l_1} \times \eta_{l_2}]^L \times [\xi_{l'_1} \times \xi_{l'_2}]^L \right]_0^0 \right\}, \end{aligned} \quad (56.1)$$

where $|2lm\rangle$ is an harmonic oscillator state of two quanta so that l is restricted to the values $l = 0, 2$, and in the last part of (56.1) we recoupled bra and ket to a total L assuming of course that V_{12} is invariant under rotations.

If the matrix elements in (56.1) are real, as happens for example when $V_{12} = V(|\mathbf{r}_1 - \mathbf{r}_2|)$, then a brief examination of it indicates that we have only seven types of independent Hermitian interactions that we proceed to write down in the notation (52.4,5)

$$A_L = \left[[\eta \times \eta]^L \times [\xi \times \xi]^L \right]_0^0, \quad L = 0, 2, 4, \quad (56.2a)$$

$$B = \left[\eta \times \xi \right]_0^0 \bar{\eta} \bar{\xi}, \quad (56.2b)$$

$$C = \bar{\eta}^2 \bar{\xi}^2, \quad (56.2c)$$

$$D = \left[\eta \times \eta \right]_0^0 \bar{\xi}^2 + \bar{\eta}^2 \left[\xi \times \xi \right]_0^0, \quad (56.2d)$$

$$E = \left[[\eta \times \eta]^2 \times \xi \right]_0^0 \bar{\xi} + \bar{\eta} [\eta \times [\xi \times \xi]]_0^0. \quad (56.2e)$$

The $A_L, L = 0, 2, 4$, are the independent interactions involving only d bosons, that can be expressed in terms of $\hat{N}^2, \hat{N}, \mathcal{L}^2$ and \hat{L}^2 . The B, C can obviously be expressed in terms of \hat{N}, \hat{N} of (45.5) and (52.8) while D is related with the \mathcal{K}^2 of (53.11) and thus with $\mathbb{L}^2 - \mathcal{L}^2$. There remains then the problem of E for which we first consider the operator $\mathcal{Q}^2 = \sum_m (-1)^m \mathcal{Q}_m \mathcal{Q}_{-m}$ taking for \mathcal{Q}_m the expression (53.19), i.e.,

$$\begin{aligned} \mathcal{Q}^2 &= \sqrt{5} [\mathcal{Q} \times \mathcal{Q}]_0^0 = \sqrt{5} \left\{ \frac{7}{3} \left[[\eta \times \xi]^2 \times [\eta \times \xi]^2 \right]_0^0 \right. \\ & \quad \left. + \frac{4}{3} \sqrt{7} \left[[\eta \times \xi]^2 \times (\eta \bar{\xi} + \bar{\eta} \xi) \right]_0^0 \right\} \end{aligned}$$

$$+ \frac{4}{3} \left[(\eta \bar{\xi} + \bar{\eta} \xi) \times (\eta \bar{\xi} + \bar{\eta} \xi) \right]_0^0. \quad (56.3)$$

Straightforward recoupling then shows that \mathcal{Q}^2 takes the form

$$\begin{aligned} \mathcal{Q}^2 = & \frac{35}{3} \sum_L \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ 2 & 2 & L \end{array} \right\} \sqrt{2L+1} A_L + \frac{7}{3} \hat{N} + \frac{4}{3} \sqrt{35} E \\ & + \frac{4}{3} [2\hat{N}(\hat{N}-\hat{N}+1) + 2(\hat{N}+5)(\hat{N}-\hat{N}) - K^2], \end{aligned} \quad (56.4)$$

where \hat{N} , \hat{N} , and K^2 are given respectively by (45.5), (52.8) and (53.11) and $\{ \}$ is a $6j$ symbol. We can then express E in terms of \mathcal{Q}^2 and the other Casimir operators of the groups in the chains mentioned in section 53. In the following equations we give explicitly the form of all the interactions (56.2) in terms of the Casimir operators mentioned:

$$A_0 = \frac{1}{5} \hat{N}(\hat{N}+3) - \frac{1}{5} \mathcal{L}^2 \quad (56.5a)$$

$$A_2 = \frac{1}{7\sqrt{5}} \left\{ -\hat{L}^2 + 2\mathcal{L}^2 + 2\hat{N}(\hat{N}-2) \right\}, \quad (56.5b)$$

$$A_4 = \frac{1}{7} \left\{ \frac{1}{3}\hat{L}^2 - \frac{1}{5}\mathcal{L}^2 + \frac{6}{5}\hat{N}(\hat{N}-2) \right\} \quad (56.5c)$$

$$B = \frac{1}{\sqrt{5}}(\hat{N}-\hat{N})\hat{N}, \quad (56.5d)$$

$$C = (\hat{N}-\hat{N})(\hat{N}-\hat{N}-1), \quad (56.5e)$$

$$D = \frac{1}{\sqrt{5}} \left\{ \mathcal{L}^2 - \mathbb{L}^2 + 2\hat{N}\hat{N} - 2\hat{N}^2 + 5\hat{N} - 4\hat{N} \right\}, \quad (56.5f)$$

$$E = \frac{3}{4\sqrt{35}} \left\{ \mathcal{Q}^2 - \frac{2}{3}\mathcal{L}^2 + \frac{4}{3}\mathbb{L}^2 - \frac{1}{6}\hat{L}^2 + \frac{14}{3}\hat{N}^2 \right. \quad (56.5g)$$

$$\left. + \frac{22}{3}\hat{N} - \frac{8}{3}\hat{N}(2\hat{N}+5) \right\}. \quad (56.5h)$$

From the discussion in the previous section it is clear that we can write the matrix elements of an arbitrary interaction in the basis of states (54.4) characterized by the irreducible representations of the chain of groups $U(6) \supset U(5) \supset O(5) \supset O(3)$. From a numerical standpoint the only stumbling block is the matrix element (55.12) of \mathcal{Q}^2 for which the reduced $3j$ symbols $(112, \kappa's'L', \kappa''s''L'')$, $(212, \kappa's'L', \kappa''s''L'')$ of $O(5)$, have been programmed. There is though a way for getting the matrix element of E directly which we proceed to discuss.

For this last task we use the definitions (56.4) and properties of the $3j$ symbols of $O(3)$ to show that

$$\begin{aligned} 2\sqrt{2} \left[[\alpha \times \alpha]^2 \times \alpha \right]_0^0 = & \\ \left[[\eta \times \eta]^2 \times \eta \right]_0^0 + 3 \left[[\eta \times \eta]^2 \times \xi \right]_0^0 \\ + 3 \left[[\xi \times \xi]^2 \times \eta \right]_0^0 + \left[[\xi \times \xi]^2 \times \xi \right]_0^0. \end{aligned} \quad (56.6)$$

Taking the matrix elements of this identity with respect to states (48.17) with ν and $\nu+1$ quanta of energy, we deduce

$$\begin{aligned} \langle \nu+1, \kappa's'LM | \left[[\eta \times \eta]^2 \times \xi \right]_0^0 | \nu\kappa sLM \rangle & \\ = -\frac{4}{3\sqrt{35}} \langle \nu+1, \kappa's'LM | \beta^3 \cos 3\gamma | \nu\kappa sLM \rangle, \end{aligned} \quad (56.7)$$

where we have used

$$\left[[\alpha \times \alpha]^2 \times \alpha \right]_0^0 = \frac{1}{\sqrt{35}} \{3,0\} = -\sqrt{\frac{2}{35}} \beta^3 \cos 3\gamma. \quad (56.8)$$

The matrix element on the right side of (56.7) factorizes into a product of the matrix elements of β^3 with respect to the functions (44.31), for which a closed formula is known [6], times the matrix element of $\cos 3\gamma$ with respect to the functions (54.16), this being proportional to the reduced $3j$ symbol $(310, \kappa's'L', \kappa sL)$ of $O(5)$ defined in (49.17) and for which computer programs are available [8,9].

Note that in the E of Eq. (56.2e) there is besides the operator appearing in (56.7), one of the form $[\eta \times [\xi \times \xi]^2]_0^0$, but as it is the hermitian conjugate of the previous one, it can also be calculated using (56.7).

Furthermore, as the calculation of the matrix elements of E in the BIR of the chain (53.2), is easier than that of \mathcal{Q}^2 done in section 55, we could use the relation (56.4) to obtain more directly the matrix elements (55.12).

Finally we would like to stress that the matrix elements of \mathcal{Q}_m , $m = 2, 1, 0, -1, -2$ given by (55.6), would be those required to calculate quadrupole transitions, i.e., $B(E2)$ in the IBM, and they can be immediately obtained from those of $\alpha_m, [\alpha \times \alpha]_m^2$ discussed in section 49.

57 Applications of the Interacting Boson Model to Problems of Nuclear Structure

So far we have developed the formalism that would allow us to calculate the matrix of the most general Hamiltonian of the IBM. The diagonalization

of this matrix will provide us with the energy levels of particular nuclei associated with a given number of bosons, *i.e.*, with a definite value of N .

We note first that if a nuclear Hamiltonian is characterized by the Casimir operators of one of the given chains of groups discussed in section 53, then our matrix would already be diagonal and the energy levels can be obtained in closed form. Thus we first consider this type of spectra writing down the chain of groups, the explicit Hamiltonian and its corresponding eigenvalue.

If we are dealing with the chain

$$\begin{matrix} U(6) & \supset & U(5) & \supset & O(5) & \supset & O(3) \\ N & & \nu & & \kappa & & L \end{matrix}, \quad (57.1)$$

where below each group we write the corresponding index of the irreducible representation, then we could consider the Hamiltonian

$$\hat{\mathcal{H}} = E_0 + \alpha \hat{N} + \beta \hat{N}^2 + \gamma \hat{N} \hat{N} + \delta \hat{L}^2 + \epsilon \hat{L}^2, \quad (57.2)$$

where $E_0, \alpha, \beta, \gamma, \delta, \epsilon$ are appropriate constants, and the energy associated with the indices in (57.1) is given by

$$E_{N\nu\kappa L} = E_0 + \alpha\nu + \beta\nu^2 + \gamma N\nu + \delta\kappa(\kappa+3) + \epsilon L(L+1). \quad (57.3)$$

For the chain

$$\begin{matrix} U(6) & \supset & O(6) & \supset & O(5) & \supset & O(3) \\ N & & \varrho & & \kappa & & L \end{matrix}, \quad (57.4)$$

the Hamiltonian could be written as

$$\mathcal{H}' = E'_0 + \alpha' \hat{L}^2 + \beta' \hat{L}^2 + \gamma' \hat{L}^2, \quad (57.5)$$

where $E'_0, \alpha', \beta', \gamma'$ are appropriate constants and the energy associated with the indices in (57.4) becomes

$$E'_{\varrho\kappa L} = E'_0 + \alpha' \varrho(\varrho+4) + \beta' \kappa(\kappa+3) + \gamma' L(L+1). \quad (57.6)$$

Finally for the chain

$$\begin{matrix} U(6) & \supset & U(3) & \supset & O(3) \\ N & & (\lambda, \mu) & & L \end{matrix}, \quad (57.7)$$

the Hamiltonian becomes

$$\mathcal{H}'' = E''_0 + \alpha'' \hat{Q}^2 + \beta'' \hat{L}^2, \quad (57.8)$$

where E''_0, α'', β'' are appropriate constants and the energy associated with the indices in (57.7), becomes

57. APPLICATIONS OF THE INTERACTING

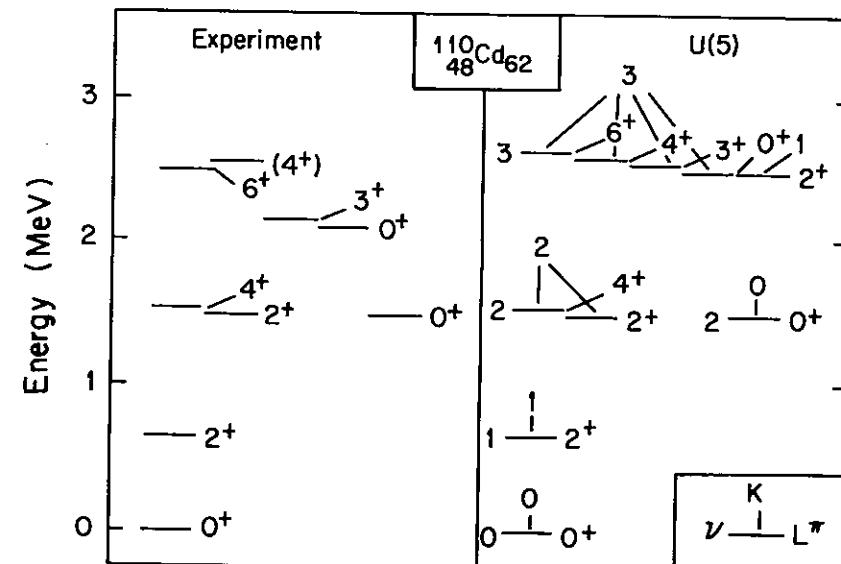


Figure X.2. Partial U(5) spectrum of the energy levels given by Eq. (57.3), where the total number of bosons is $N = 7$, and its comparison with those observed for the nucleus $^{110}_{48}\text{Cd}$. The calculated spectrum is obtained with the parameters (in keV), $[\alpha + (\gamma/7)] = 156$, $\beta = 97$, $\delta = -2.5$, $\epsilon = 5$, with the energy of the ground state normalized to 0. Levels are labeled by ν, κ and the angular momentum and parity L^π . Taken from *Algebraic methods in molecular and nuclear structure physics* by A. Frank and P. van Isacker, John Wiley and Sons Inc. (reprinted by permission; ref. [2]).

$$\begin{aligned} E''_{\lambda\mu L} = & E''_0 + \beta'' L(L+1) \\ & + \frac{\alpha''}{10} \left[(\lambda+2\mu)(\lambda+2\mu+6) + 3\lambda(\lambda+2) - 7L(L+1) \right], \end{aligned} \quad (57.9)$$

where we made use of Eqs. (39.7)–(39.9).

The energies $E_{N\nu\kappa L}$ of (57.3) are applied to the description of the spectrum of $^{110}_{48}\text{Cd}$ which is of a vibrational type, and where there are $N = 7$ bosons. The theoretical spectra [2], where the values ν, κ, L are indicated, appear in Fig. X.2, where also the experimental levels are given. The values of the parameters $E_0, \alpha, \beta, \gamma, \delta, \epsilon$ are in the caption of Fig. X.2.

The energies $E'_{\varrho\kappa L}$ of (57.6) are applied to the discussion of the spectrum of $^{196}_{78}\text{Pt}_{118}$, which is a γ unstable nucleus, and where $N = 6$ bosons. The theoretical spectra [2] where the values ϱ, κ, L are indicated, appears in Fig. X.3, where also the experimental levels are given. The values of the parameters $E'_0, \alpha', \beta', \gamma'$, are in the caption of Fig. X.3.

Finally the energies $E''_{\lambda\mu L}$ of (57.9) are applied to the discussion of the spectrum $^{156}_{64}\text{Gd}_{92}$ which is of the rotational type, and where $N = 12$ bosons. The theoretical spectrum where the values λ, μ, L are indicated appear in Fig. X.4, where also the experimental levels are given. The values of the parameters E''_0, α'', β'' are in the caption of Fig. X.4.

We want now to discuss examples in which the full Hamiltonian of Section 56 needs to be used. A particularly interesting case is to consider an IBM Hamiltonian in which the coefficients of the seven types of interactions in (56.2) are adjusted by a least square procedure to a family of isotopes. As the number of bosons changes from isotope to isotope, one can see how with the same Hamiltonian we are passing from vibrational to rotational spectra.

We shall illustrate here the case of the Samarium isotopes where Castaños, Federman, Frank and Pittel [10] used essentially a Hamiltonian of the form

$$\hat{\mathcal{H}}_{IBM} = k_1 \hat{N} + k_2 \hat{N} \hat{N} + k_3 \hat{Q}^2, \quad (57.10)$$

and adjusted k_1, k_2, k_3 by a least square fit for all the levels between ^{148}Sm and ^{154}Sm and showed how, by the changes in N , one passes from a vibrational spectrum in ^{148}Sm to a rotational one in ^{154}Sm as illustrated in Fig. X.5. The matrix elements of $\hat{\mathcal{H}}_{IBM}$ of (57.10) were calculated in the BIR associated with $U(6) \supset U(5) \supset O(5) \supset O(3)$, by the type of procedures outlined in this chapter.

A similar analysis, with a somewhat more general Hamiltonian than (57.10), was done for other chains of isotopes by the authors referred above [10] and we illustrate their results in the case of uranium going from ^{230}U to ^{238}U in Fig. X.6. In both Figs. X.5 and X.6 the theoretical energy levels are compared with the experimental ones.

As in section 50, we could also calculate with the states discussed in this chapter, the quadrupole transitions, but as the analysis is similar to the one we carried out in the previous chapter, we do not consider it worthwhile to discuss them here.

A much more detailed analysis of the IBM and its generalizations, is given in part III of the book [2] by Frank and Van Isacker.

We would like to finish by indicating that the techniques developed in Chapters IX and X of this book also have relevance to the discussion of microscopic descriptions of collective motions in nuclei, as discussed in reference [11].

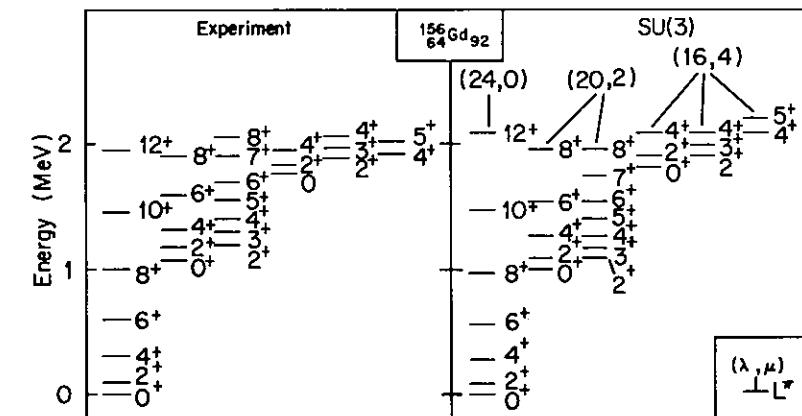
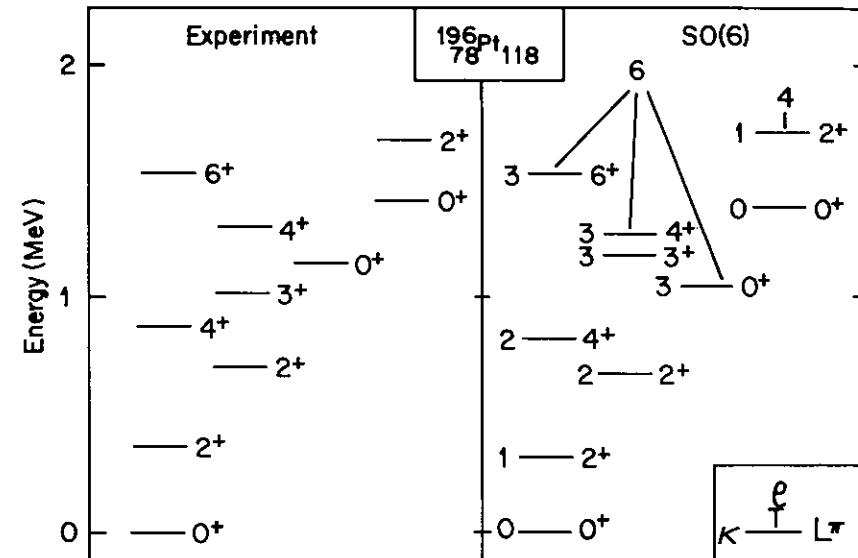


Figure X.3 (top). Partial O(6) spectrum of the energy levels given by (57.6) for $N = 6$ bosons and its comparison with the observed levels of the nucleus ^{196}Pt . The calculated spectrum is obtained with the parameters (in keV) $\alpha' = -50, \beta' = 58, \gamma' = 11$, with the energy of the ground state normalized to zero. Levels are labeled by ρ, κ and the angular momentum and parity L^π . Taken from *Algebraic methods in molecular and nuclear structure physics* by A. Frank and P. van Isacker, John Wiley and Sons Inc. (reprinted by permission, ref. [2]).

Figure X.4 (bottom). Partial SU(3) spectrum of the energy levels given by (57.9) for $N = 12$ bosons and its comparison to the observed levels of the nucleus ^{156}Gd . The calculated spectrum is obtained with the parameters (in keV) $\alpha'' = -17.5, \beta'' = 7.75$, and with the energy of the ground state normalized to zero. Levels are labeled by (λ, μ) and the angular momentum and parity L^π .

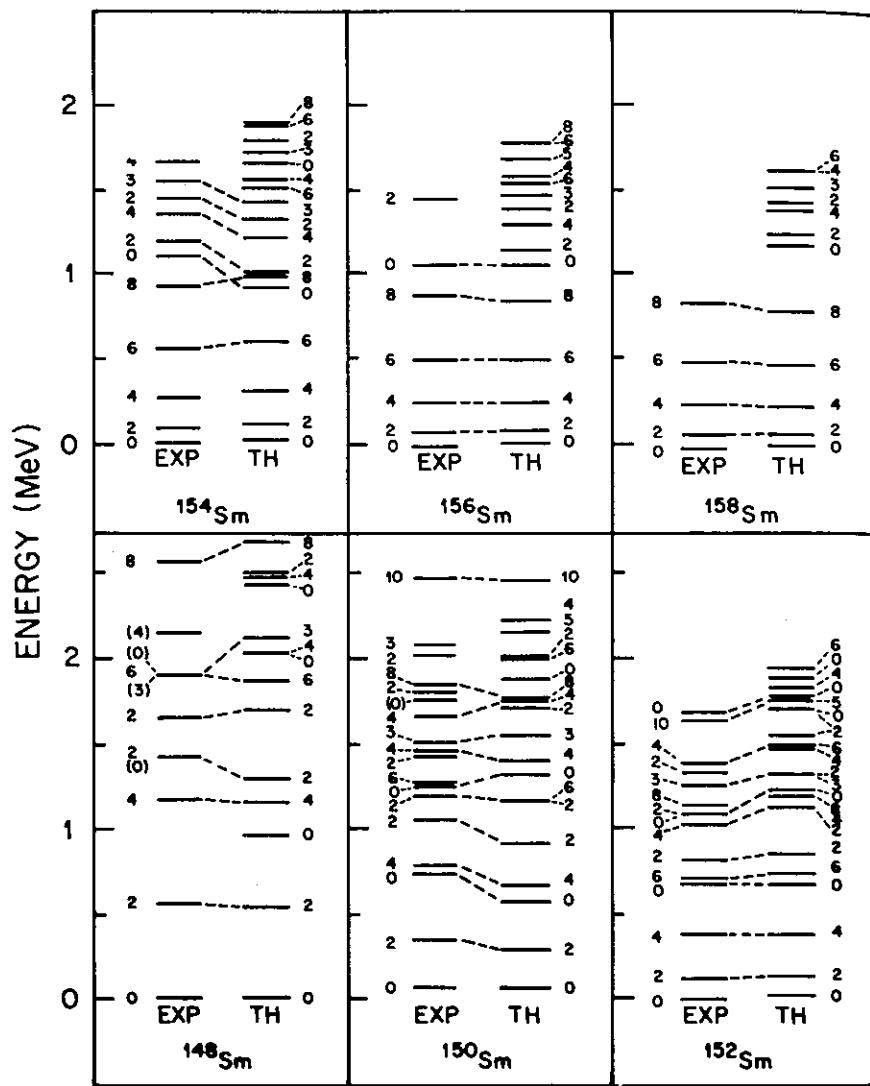


Figure X.5. Comparison of experimental and theoretical levels of the Sm isotopes. The analysis was done employing the techniques described in §57 of this book for calculations in the IBM. Experimental spins in parenthesis indicate tentative assignments. Experimental and theoretical levels connected by dashed lines were included in the least square fit. Taken from O. Castaños, A. Frank, and P. Federman, reference [10].

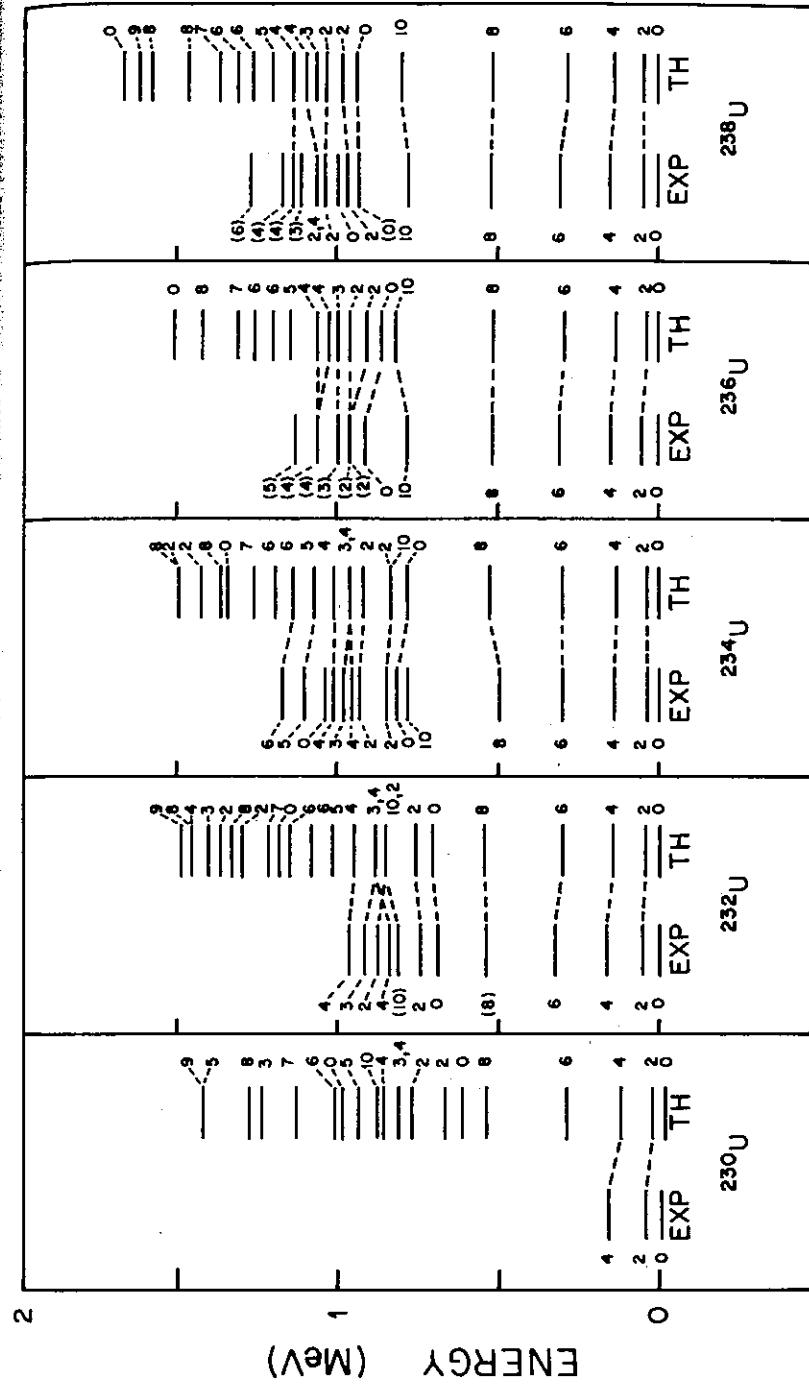


Figure X.6. Comparison of the experimental and theoretical levels in the U isotopes. The notation is the same as in Fig. X.5. Taken from O. Castaños, A. Frank, P. Federman and S. Pittel, ref. [10].

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Chapter XI

The One-Body Relativistic Oscillator

The harmonic oscillator was one of the first examples on which the ideas of quantum mechanics were tried, both in the old and in the present version of this theory.

Thus, besides its innumerable applications in problems of nonrelativistic quantum mechanics, some of which have been treated in the previous chapters of this book, it also contributed to the birth of this formalism.

Since the late twenties the physicists found themselves in possession not only of quantum mechanics, but also of the theory of relativity, and had the problem of achieving a happy marriage of the two. Almost seventy years later, and after many papers and books, we seem still far from the objective mentioned.

In the next three chapters we will try to deal with the problem from the standpoint of the simplest interaction, *i.e.*, the harmonic oscillator. We shall concentrate on the relativistic *quantum mechanics* of one or many bodies with harmonic oscillator interactions but not on relativistic quantum *field theories*. The latter subject, which may be more physically significant, but also much more complex mathematically, is outside the scope of this book. Nevertheless the problems with which we shall deal here may sharpen our intuition on systems in which quantum mechanics and relativity are interrelated and even, if we restrict ourselves to the positive energy part of resulting spectra, may give some insight on the masses of baryons and mesons.

We shall start in this chapter with the one-body relativistic problem in a scalar or spinor form, for which different aspects of an oscillator interaction

can be considered. While we shall discuss these problems in a particular frame of reference we also show that they can be formulated in a Lorentz invariant form.

At the beginning of the following chapters we shall indicate their content for relativistic two and n -body problems, though in the latter case we shall concentrate on $n = 3$.

We start with the scalar one-body relativistic oscillator.

58 The Klein-Gordon Equation with an Oscillator Interaction

It is convenient first to define our variables and notation. We shall designate our covariant space time coordinates as

$$x^\mu, \quad \mu = 0, 1, 2, 3, \quad (58.1)$$

with $x^0 = t$, being the time variable, while x^i , $i=1,2,3$, are the components of the space vector. Later, when we will deal with n particles, we shall add a lower index $s = 1, 2, \dots, n$. Our metric tensor $g_{\mu\nu}$ will have the values

$$g_{\mu\nu} = 0 \quad \text{if } \mu \neq \nu, \quad -g_{00} = g_{11} = g_{22} = g_{33} = 1, \quad (58.2)$$

so the covariant form of our coordinates x_μ is related with the contravariant ones by

$$x_\mu = g_{\mu\nu} x^\nu; \quad x_0 = -x^0, \quad x_i = x^i, \quad i = 1, 2, 3, \quad (58.3)$$

where repeated greek indices will always indicate summation over their values $\nu = 0, 1, 2, 3$. Note that the contravariant form $g^{\mu\nu}$ of the metric tensor has also the definition (58.2).

We shall use units in which

$$\hbar = m = c = 1, \quad (58.4)$$

where m is the mass which, in these last three chapters, will be assumed equal for all the particles involved, and c is the velocity of light. Note that this is different from the previous chapters where we took $\hbar = m = \omega = 1$, so the frequency of the oscillator ω is a parameter that will appear explicitly in our equations.

The momenta in this space time will be defined as

$$p_\mu = \frac{1}{i} \frac{\partial}{\partial x^\mu} \quad \text{or} \quad p^\mu = \frac{1}{i} \frac{\partial}{\partial x_\mu}, \quad (58.5)$$

so that the free particle Klein-Gordon equation, in the units (58.4) can be written as

$$[g^{\mu\nu} p_\mu p_\nu + 1] \Psi = \left[-g^{\mu\nu} \frac{\partial^2}{\partial x^\mu \partial x^\nu} + 1 \right] \Psi = 0. \quad (58.6)$$

How to introduce an oscillator interaction in this equation? One obvious way is to consider an additional term,

$$\omega^2 g^{\mu\nu} x_\mu x_\nu, \quad (58.7)$$

in the square bracket. This would give rise to beautiful mathematical problems for which the symmetry Lie algebra will be $u(3,1)$ and we could consider the solution in the chain [1]

$$U(3,1) \supset O(3,1) \supset O(3) \supset O(2), \quad (58.8)$$

where $O(3,1)$ is the Lorentz group. This has been done by several authors [1] in the simpler case when the space is one rather than three dimensional, i.e., $U(1,1) \supset O(1,1)$, but even then it is a complex problem. Discussions have also been given [2] for the chain (58.8).

We shall not follow this path as it involves (as can be clearly seen trivially when the problem is solved in cartesian coordinates) vibrations in the time axis [2] to which no clear significance can be attached.

Rather we shall start by assuming that there is an harmonic oscillator potential acting on the particle in some *definite* frame of reference and worry later about the Lorentz invariance of the problem. Thus we get the equation

$$\left[\frac{\partial^2}{\partial x^{02}} - \nabla^2 + \omega^2 r^2 + 1 \right] \Psi = 0. \quad (58.9)$$

As there is no dependence on time of the potential in this formulation of the problem we can propose a solution of the form

$$\Psi = \psi \exp(-iEx^0), \quad (58.10)$$

which leads us to the equation

$$(-\nabla^2 + \omega^2 r^2 + 1)\psi = E^2 \psi, \quad (58.11)$$

almost identical to (1.1). From (1.2) and (1.8) the solution can be written as

$$\psi_{nlm}(\mathbf{x}) \equiv |nlm\rangle = R_{nl}(\sqrt{\omega}r) Y_{lm}(\theta, \varphi), \quad (58.12)$$

where, because of the presence of ω^2 in (58.11), our radial function depends on $\sqrt{\omega r}$ instead of r . For the same reason we now get instead of (1.7) that

$$E_N^2 = 1 + 2\omega(2n + \ell + \frac{3}{2}) = 1 + \omega(2N + 3), \quad (58.13)$$

where we introduced an index N for the energy defined by

$$N = 2n + \ell. \quad (58.14)$$

If N is fixed then ℓ can take the value $N, N-2, \dots, 0$ or 1 . The problem is then very simple and, in fact, if $\omega \ll 1$, i.e., the nonrelativistic limit, E_N will be close to 1 so we can write

$$E_N^2 - 1 = (E_N - 1)(E_N + 1) \simeq 2(E_N - 1) \equiv 2\epsilon_N, \quad (58.15)$$

where ϵ_N is defined as $\epsilon_N = E_N - 1$ and thus we get $\epsilon_N = \omega(N + \frac{3}{2})$ as we should expect from (1.7).

The reason we discuss this trivial problem is that it shows a type of behavior that we will also find in more complex situations, as well as those involving more particles but, besides, because we proceed to write it in a Lorentz invariant form.

For the latter purpose we define a *unit, time like, four vector* u_μ , $\mu = 0, 1, 2, 3$, which thus has the property that in some space time frame of reference it has the form

$$(u_\mu) = (1, 0, 0, 0). \quad (58.16)$$

In all other frames it can be obtained by applying to its form in (58.16) a boost, i.e., a Lorentz transformation, as well as any required rotations.

With the help of this u_μ we can now define the transverse part of the position space time vector x^μ , which we designate as x_\perp^μ , as

$$x_\perp^\mu \equiv x^\mu + (x^\nu u_\nu) u^\mu. \quad (58.17)$$

This implies that in the frame of reference where (u_ν) takes the form (58.16) and where, because of our metric, $(u^\mu) = (-1, 0, 0, 0)$ we have

$$x_\perp^0 = 0, \quad x_\perp^i = x^i, \quad i = 1, 2, 3. \quad (58.18)$$

Thus a Lorentz invariant equation corresponding to (58.9) can be written as

$$\left[-g^{\mu\nu} \frac{\partial^2}{\partial x^\mu \partial x^\nu} + \omega^2 g^{\mu\nu} x_{\perp\mu} x_{\perp\nu} + 1 \right] \Psi = 0, \quad (58.19)$$

as in the frame of reference where (u_μ) takes the form (58.16) it becomes identical to (58.9).

We can now ask how does the solution of our problem, given by (58.10, 12), looks in an arbitrary frame of reference where the vector (u_μ) can be written as

$$(u_\mu) = (u_0, \mathbf{u}), \quad (58.20)$$

where u_0 is the temporal part and \mathbf{u} is a three-dimensional vector corresponding to the spatial part. Comparing Eq. (58.20) and (58.16), we see that we require a transformation of space time coordinates $(x_\mu) = (x_0, \mathbf{x})$ by a boost in the direction of the vector \mathbf{u} .

To write explicitly the boost transformation we note first that from (58.16) and (58.20) we have

$$g^{\mu\nu} u_\mu u_\nu = -u_0^2 + (\mathbf{u} \cdot \mathbf{u}) = -1, \quad (58.21)$$

so we could designate $|u_0|$ and $(\mathbf{u} \cdot \mathbf{u})^{1/2}$ as

$$|u_0| = \cosh h\delta \equiv c, \quad (58.22a)$$

$$(\mathbf{u} \cdot \mathbf{u})^{\frac{1}{2}} = |\sin h\delta| \equiv s, \quad (58.22b)$$

with δ being an arbitrary real parameter as, in this way, Eq. (58.21) will always be satisfied. Note that now

$$(\mathbf{u}/s) \quad (58.23)$$

will be a unit vector in the three-dimensional space.

To express explicitly this boost we have to decompose the three vector \mathbf{x} into its parts parallel and orthogonal to the vector \mathbf{u} , and then carry out a Lorentz transformation involving the orthogonal part and x_0 . Thus we arrive at a new space time coordinate $(x'_\mu) = (x'_0, \mathbf{x}')$ given by

$$\begin{aligned} \mathbf{x}' &= [\mathbf{x} - s^{-2}(\mathbf{x} \cdot \mathbf{u})\mathbf{u}] \\ &\quad + [(c/s)(\mathbf{x} \cdot \mathbf{u}) - sx_0](\mathbf{u}/s), \end{aligned} \quad (58.24a)$$

$$x'_0 = cx_0 - (\mathbf{u} \cdot \mathbf{x}). \quad (58.24b)$$

Equation (58.24) is what is known as a *passive* Lorentz transformation [3] from the old space time variables (x_0, \mathbf{x}) to the new ones (x'_0, \mathbf{x}') caused by a boost associated with the four vector (u_0, \mathbf{u}) . On the other hand if we replace in Eq. (58.24) the (x_0, \mathbf{x}) by (u_0, \mathbf{u}) of (58.20) we immediately see that it leads to the four vector $(1, 0, 0, 0)$ of (58.16). This is an *active* Lorentz

transformation [3] from the new to the old (u_μ) and, as we should expect, it acts in the inverse sense of the *passive* one.

The effect of the boost on the wave function (58.10,12) is to replace x_0, r, θ, φ which are functions of (x_0, \mathbf{x}) , by the corresponding ones in (x'_0, \mathbf{x}') , and then use Eq. (58.24) to recover them in the original space time. To show physically what this procedure implies we consider a simple case of the wave function (58.10,12) in which $n = \ell = 0$, so Ψ becomes

$$\begin{aligned}\Psi(x_0, \mathbf{x}) &= \omega^{3/2} \pi^{-3/4} \exp[-(\omega/2)(x_1^2 + x_2^2 + x_3^2)] \\ &\quad \exp[-i(1+3\omega)^{1/2}x_0].\end{aligned}\quad (58.25)$$

We then wish to express it in the space time coordinates in which the unit time like four vector becomes

$$(u_\mu) = (c, s, 0, 0), \quad (58.26)$$

i.e., the boost is the direction of x_1 , so Eq. (58.24) reduces to

$$x'_1 = cx_1 - sx_0, \quad x'_2 = x_2, \quad x'_3 = x_3, \quad x'_0 = cx_0 - sx_1. \quad (58.27)$$

Replacing then (x_0, \mathbf{x}) in (58.25) by (x'_0, \mathbf{x}') and using (58.27) we obtain that the new wave function, in the old coordinates, which we designate by Ψ' takes the form

$$\begin{aligned}\Psi'(x_0, \mathbf{x}) &= \omega^{3/2} \pi^{-3/4} \exp\{-(\omega/2)[(cx_1 - sx_0)^2 + x_2^2 + x_3^2]\} \\ &\quad \times \exp[-i(1+3\omega)^{1/2}(cx_0 - sx_1)].\end{aligned}\quad (58.28)$$

In particular, the probability density $|\Psi'|^2$, which is the physically relevant quantity, becomes

$$|\Psi(x_0, \mathbf{x})|^2 = \omega^3 \pi^{-3/2} \exp[-\omega(x_1^2 + x_2^2 + x_3^2)] \quad (58.29)$$

in the frame of reference where (u_μ) takes the form (58.16), while it is given by

$$|\Psi'(x_0, \mathbf{x})|^2 = \omega^3 \pi^{-3/2} \exp[-(\omega c^2)(x_1 - \frac{s}{c}x_0)^2 - \omega(x_2^2 + x_3^2)] \quad (58.30)$$

in the frame of reference where (u_μ) takes the value (58.26).

In the first case we have a spherical Gaussian with center at the origin whose width is $\omega^{-1/2}$, while in the second it is an oblate Gaussian whose width is still $\omega^{-1/2}$ in the directions x_2, x_3 , but it becomes $\omega^{-1/2}c^{-1}$ in the direction x_1 . Furthermore for a fixed time x_0 , the center of this oblate ellipsoidal Gaussian has moved from $x_i = 0, i = 1, 2, 3$ to $x_1 = (\tanh \delta)x_0, x_2 = x_3 = 0$, and, if (u_μ) of Eq. (58.20) would be interpreted as a four momentum, $(\tanh \delta)$ would be its corresponding velocity. Thus we get an intuitive feeling of the effect on the wave function of the vector (u_μ) , i.e., in this case a contraction in the x_1 direction as $c > 1$ and a displacement of x_1 by an appropriate velocity multiplied by the time x_0 .

59 The Dirac Oscillator

If we consider Eq. (58.9) with $\omega = 0$, we have, in our units, the standard Klein-Gordon equation, and we know that the great achievement of Dirac was to linearize it to get the equation that bears his name:

$$i \frac{\partial \psi}{\partial x^0} = (\alpha \cdot \mathbf{p} + \beta)\psi, \quad (59.1)$$

where \mathbf{p} is the ordinary three-dimensional momentum, i.e., $p_i = -i\partial/\partial x_i$, $i = 1, 2, 3$ and α and β are the 4×4 matrices

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad (59.2a)$$

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (59.2b)$$

with σ being the vector whose components $\sigma_i, i = 1, 2, 3$ are the 2×2 Pauli spin matrices and I is 2×2 unit matrix.

What would be the corresponding result when we want to linearize Eq. (58.9) but with $\omega \neq 0$? This is the question that Moshinsky and Szczepaniak [4] asked themselves in 1989, and arrived at the conclusion that it could be an equation linear in both \mathbf{p} and \mathbf{r} that in fact could be written as

$$i(\partial \psi / \partial x^0) = [\alpha \cdot (\mathbf{p} - i\omega \mathbf{r}\beta) + \beta]\psi, \quad (59.3)$$

and they baptized it with the name of the Dirac oscillator [4].

It was found later that Ito *et al.* and Cook [5] had arrived earlier, by a different reasoning, to this type of equation, but the development of the idea stopped with them, while the Dirac oscillator concept [4] has already given rise to dozens of papers.

We now proceed to solve Eq. (59.3) by proposing a ψ of the form

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \exp(-iEx^0), \quad (59.4)$$

where, for positive energy E , ψ_1, ψ_2 are the large and small component of the wave function, depending only on the spatial coordinates and satisfying the equations

$$(E - 1)\psi_1 = \sigma \cdot (\mathbf{p} + i\omega \mathbf{r})\psi_2, \quad (59.5a)$$

$$(E + 1)\psi_2 = \sigma \cdot (\mathbf{p} - i\omega \mathbf{r})\psi_1. \quad (59.5b)$$

Multiplying the first equation by $(E + 1)$ and using the second we arrive finally that ψ_1 satisfies

$$(E^2 - 1)\psi_1 = (p^2 + \omega^2 r^2 - 3\omega - 4\omega \mathbf{L} \cdot \mathbf{S})\psi_1, \quad (59.6)$$

where

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad \mathbf{S} = (\sigma/2), \quad (59.7)$$

are the orbital and spin angular momenta.

If the spin would have been $s = 0$, this would have been, except for an irrelevant constant, exactly Eq. (58.11), so we see that the harmonic oscillator eigenstate $|nlm\rangle$ of (50.12), would have been a solution. If we have spin 1/2, though, we have to couple it with the orbital part to give a state of total angular momentum:

$$\mathbf{J} = \mathbf{L} + \mathbf{S}. \quad (59.8)$$

These can be achieved with the help of a $3j$ coefficient, thus providing us with the solution

$$\begin{aligned} \psi_1 = |N(\ell, \frac{1}{2})jm\rangle &= \sum_{\mu, \sigma} \sqrt{2j+1}(-1)^{\ell-\frac{1}{2}+m} \\ &\times \begin{pmatrix} \ell & \frac{1}{2} & j \\ \mu & \sigma & -m \end{pmatrix} R_{N\ell}(\sqrt{\omega}r) Y_{\ell\mu}(\theta, \varphi) \chi_{\sigma}, \end{aligned} \quad (59.9)$$

where we have made use of (58.12) and of a spinor function χ_{σ} , corresponding to the value 1/2 for the spin with projection $\sigma = \pm(1/2)$.

As the ket (59.9) is an eigenfunction of $p^2 + \omega^2 r^2, L^2, S^2, J^2$, and the spin orbit coupling $\mathbf{L} \cdot \mathbf{S}$ can be written as

$$\mathbf{L} \cdot \mathbf{S} = (1/2)(J^2 - L^2 - S^2), \quad (59.10)$$

we see that the eigenvalues of the energy E depend on the number of quanta $N = 2n + \ell$ of (58.14), on the total angular momentum which we denote by j , and on the orbital one ℓ , so we could write it as $E_{N\ell j}$ and from Eq. (59.6) we see that these eigenvalues take the form

$$E_{N\ell j}^2 = 1 + \omega \begin{cases} [2(N-j)+1] & \text{if } \ell = j - \frac{1}{2} \\ [2(N+j)+3] & \text{if } \ell = j + \frac{1}{2} \end{cases}. \quad (59.11)$$

At first sight the energy spectrum of this problem looks similar to the Klein-Gordon oscillator of (58.13), but actually it is very different. When $\ell = j - \frac{1}{2}$, we have an infinite accidental degeneracy, as all pairs

$$(N, j), \quad (N \pm 1, j \pm 1), \quad (N \pm 2, j \pm 2), \dots, \quad (59.12)$$

have the same value of the energy. On the other hand if $\ell = j + \frac{1}{2}$, the pairs that guarantee the same energy are

$$(N, j), \quad (N \pm 1, j \mp 1), \quad (N \pm 2, j \mp 2), \dots, \quad (59.13)$$

and the series ends when $N = 0$ or $j = 1/2$, which indicates that we have a finite degeneracy.

In the Klein-Gordon oscillator, like in the ordinary one, the degeneracy

$$\frac{1}{2}(N+1)(N+2) \quad (59.14)$$

is explained by a $u(3)$ symmetry Lie algebra as was shown in Chapter VII.

For this Dirac oscillator the situation is more complex and Quesne and Moshinsky [6] showed that the degeneracy is explained by $so(4) \otimes so(3,1)$ Lie algebra whose generators will be indicated in subsection a) of this Chapter.

Note that the expression (59.9) is a solution only for the large component ψ_1 in Eq. (59.5), while the small one is given by

$$\begin{aligned} \psi_2 &= (E_{N\ell j} + 1)^{-1} [\sigma \cdot (\mathbf{p} - i\omega \mathbf{r})] \psi_1 \\ &= (E_{N\ell j} + 1)^{-1} [-i(2\omega)^{1/2}] (\sigma \cdot \xi) |N(\ell, \frac{1}{2})jm\rangle, \end{aligned} \quad (59.15)$$

where ξ will be the annihilation, and η the creation operators of the oscillator which, in the present units, i.e., $\hbar = m = c = 1$, will have the form

$$\eta = \frac{1}{\sqrt{2}}(\omega^{1/2}\mathbf{r} - i\omega^{-1/2}\mathbf{p}), \quad \xi = \frac{1}{\sqrt{2}}(\omega^{1/2}\mathbf{r} + i\omega^{-1/2}\mathbf{p}), \quad (59.16)$$

while $E_{N\ell j}$ is given by (59.11).

The presence $(\sigma \cdot \xi)$ in (59.15) implies that for ψ_2 , N is replaced by $N - 1$ while j and m remain unchanged and, because of parity ℓ goes into $\ell \pm 1$. An elementary analysis involving Racah algebra, as well as the matrix element (10.35), will then give us ψ_2 in the form

$$\begin{aligned} \psi_2 &= (E_{N\ell j} + 1)^{-1} [-i(2\omega)^{1/2}] \{ -(N+\ell+1)^{1/2} |N-1(\ell-1, \frac{1}{2})jm\rangle \\ &+ (N-\ell)^{1/2} |N-1(\ell+1, \frac{1}{2})jm\rangle \}. \end{aligned} \quad (59.17)$$

We have then the complete solution of the Dirac oscillator equation (59.3) given by (59.4,9,17), but it is valid only in a particular frame of reference in which the interaction is given by $[-i\omega(\alpha \cdot \mathbf{r})\beta]$. As in the case of the Klein-Gordon oscillator we have to write it also in a Lorentz invariant form, which we shall proceed to do in two different ways, but in both making use of the unit time like four vector (u_{μ}) in its forms (58.16) or (58.20).

In the first way we introduce the 4×4 matrix four vector γ^μ by the usual definitions [7]:

$$\gamma^i = \beta \alpha_i, \quad i = 1, 2, 3, \quad (59.18a)$$

$$\gamma^0 = \beta, \quad (59.18b)$$

and write the equation of the Dirac oscillator as

$$\{\gamma^\mu [p_\mu - i\omega x_{\perp\mu} (u^\tau \gamma_\tau)] + 1\} \psi = 0, \quad (59.19)$$

where $x_{\perp\mu}$ is defined by (58.17). Clearly then it is Lorentz invariant equation which, when (u_μ) takes the form (58.16), *i.e.*, $(u_\mu) = (1, 0, 0, 0)$, and we multiply it by β , reduces to Eq. (59.3).

In the second way, followed by Moreno and Zentella [8], one uses the antisymmetric tensor for spin [9] in the four-dimensional space time, *i.e.*,

$$S^{\mu\nu} = (i/4)(\gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu), \quad (59.20)$$

and writes the Lorentz invariant equation

$$[\gamma^\mu p_\mu + \omega S^{\mu\nu} (u_\mu x_\nu - u_\nu x_\mu) + 1] \psi = 0. \quad (59.21)$$

Again taking (u_μ) in the form (58.16), we have that the interaction term becomes

$$\omega S^{\mu\nu} (u_\mu x_\nu - u_\nu x_\mu) = 2\omega \sum_{i=1}^3 S^{0i} x_i = i\omega \gamma^0 (\gamma \cdot \mathbf{r}) = i\omega (\boldsymbol{\alpha} \cdot \mathbf{r}), \quad (59.22)$$

and, as before, multiplying by β Eq. (59.21) we recover Eq. (59.3).

The form (59.21) of the Dirac oscillator equations suggests that we can interpret it as coming from an anomalous magnetic moment, being enacted by the electromagnetic field

$$F_{\mu\nu} = u_\mu x_\nu - u_\nu x_\mu. \quad (59.23)$$

Actually the two expressions (59.19) and (59.21) for the Lorentz invariant form of Eq. (59.3) are identical, because it is easy to prove that the interaction parts in them coincide, *i.e.*,

$$-i\omega (\gamma^\mu x_{\perp\mu}) (u_\nu \gamma^\nu) = \omega S^{\mu\nu} (u_\mu x_\nu - u_\nu x_\mu), \quad (59.24)$$

if we use the definition (58.17) of $x_{\perp\mu}$ and the relations

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = -2g^{\mu\nu}, \quad (59.25a)$$

$$g^{\mu\nu} u_\mu u_\nu = -1. \quad (59.25b)$$

59. THE DIRAC OSCILLATOR

We derived though both of them, as (59.19) is more useful for comparison with relativistic many-body problems interacting through Dirac oscillators, while (59.21) has a clearer physical meaning.

We can now ask, as we did in the case of the Klein-Gordon oscillator, how does the solution (59.4,9,17) of our problem, look in an arbitrary frame of reference where the vector (u_μ) takes the form (58.20), *i.e.*, $(u_\mu) = (u_0, \mathbf{u})$.

For the space time part of the solution (59.4,9,17) the change is exactly the same as discussed in section 58 for the Klein-Gordon particle. We have though also the spinor function χ_σ in (59.9,17) and we must discuss how does it change under a boost in the direction \mathbf{u} .

For this purpose we note as γ^μ is a 4×4 matrix four vector, under a Lorentz transformation $A = \|a_\nu^\mu\|$ whose components are $a_\nu^\mu, \mu, \nu = 0, 1, 2, 3$, it becomes

$$\gamma'^\mu = a_\nu^\mu \gamma^\nu = \mathcal{U} \gamma^\mu \mathcal{U}^{-1}, \quad (59.26)$$

where on the right hand side we have put the matrices, representations of A , that carry out this transformation as required by quantum mechanics [10].

As we are only interested in boosts, we can start by considering them in the direction $\mu = 3$, *i.e.*,

$$A = \begin{pmatrix} c & 0 & 0 & s \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ s & 0 & 0 & c \end{pmatrix}, \quad (59.27)$$

with c, s given by (58.22).

Which is the \mathcal{U} corresponding to A of (59.27)? We note first that the commutation rules of $S^{\mu\nu}$ given in reference [9] indicate that they behave as the generators of a Lie algebra $o(3,1)$, *i.e.*, corresponding to the Lorentz group. The $S^{ij}, i, j = 1, 2, 3$ are associated with infinitesimal rotations, so $S^{0i} = -S^{i0}$ must be connected with infinitesimal boosts and, in particular, S^{03} is connected [9] with this type of boost in the direction $\mu = 3$.

From the definition (59.20) of $S^{\mu\nu}$, and using (59.18,2) we see that

$$S^{03} = (i/2) \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \quad (59.28a)$$

with σ_3 being the Pauli spin matrix:

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (59.28b)$$

Clearly then the finite boost of magnitude δ for the direction $\mu = 3$ will be then [9]

$$\mathcal{U} = \exp(i\delta S^{03}) = \begin{pmatrix} \bar{c}I & -\bar{s}\sigma_3 \\ -\bar{s}\sigma_3 & \bar{c}I \end{pmatrix}, \quad (59.29)$$

where

$$\bar{c} = \cosh(\delta/2), \quad \bar{s} = \sinh(\delta/2), \quad (59.30)$$

and both I and σ_3 are 2×2 matrices.

We recall from (58.23) that (u/s) is a unit three-dimensional vector in the direction u . Thus if the boost, instead of the direction $\mu = 3$, is given in an arbitrary one, we have to make the replacement

$$\sigma_3 \rightarrow (u \cdot \sigma)s^{-1}, \quad (59.31)$$

and the matrix (59.29) becomes

$$\mathcal{U} = \begin{pmatrix} \bar{c}I & -\bar{s}(\sigma \cdot u)s^{-1} \\ -\bar{s}(\sigma \cdot u)s^{-1} & \bar{c}I \end{pmatrix}, \quad (59.32)$$

while \mathcal{U}^{-1} is obtained by just changing $-\bar{s}$ to \bar{s} .

This matrix \mathcal{U} is the one that must be applied to the state (59.4), accompanied with the change (58.24) of the space time coordinates, to get the wave function in an arbitrary reference frame.

a) The symmetry Lie algebra of the Dirac oscillator

As we indicated in Eqs. (59.11–13) the energy levels of the Dirac oscillator have considerable accidental degeneracy which is interesting to explain. This was done by Quesne and Moshinsky [6] in full detail, but here we shall only discuss the main ideas involved in the procedure and give, without proof, the explicit form of the generators of the Lie algebras involved.

It is convenient first to distinguish between the energies $E_{N\ell j}$ of (59.11) when $\ell = j + \frac{1}{2}$ and $\ell = j - \frac{1}{2}$ by using the symbols

$$\epsilon_\nu \equiv (2\omega)^{-1}(E_{Nj+\frac{1}{2}j}^2 - 1) = 2\nu + 3; \quad \nu = \frac{1}{2}(N + j - \frac{3}{2}), \quad (59.33a)$$

$$\epsilon_n \equiv (2\omega)^{-1}(E_{Nj-\frac{1}{2}j}^2 - 1) = 2n; \quad n = \frac{1}{2}(N - j + \frac{1}{2}). \quad (59.33b)$$

We then indicate in Fig. XI.1 the values of ϵ_ν, ϵ_n in the ordinate, and the values of j in the abscissa, while on each level we indicate the values of N, ℓ . The levels ϵ_ν are marked by a cross while those in ϵ_n do not have one.

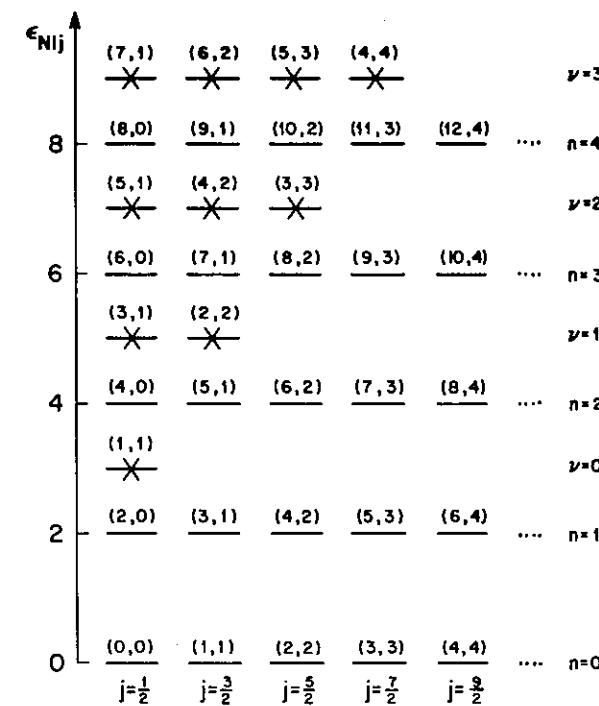


Figure XI.1. Energy spectrum of the Dirac oscillator. The abscissa corresponds to the total angular momentum and the ordinate with cross to $\epsilon_{Nl_j} = \epsilon_\nu$ and without to $\epsilon_{Nl_j} = \epsilon_n$. The values (N, l) are given above the levels. Taken from C. Quesne and M. Moshinsky, ref. [6].

It is clear that the levels ϵ_ν and ϵ_n have different type of degeneracies. For the first the j of the total angular momentum takes the finite number of values $(1/2), (3/2), \dots, (\nu + 1/2)$, and thus, as there are $(2j + 1)$ possibilities for $m = j, j - 1, \dots, -j$, for each level the total degeneracy of a state of given ν is

$$d(\nu) = \sum_{j=(1/2)}^{(\nu+1/2)} (2j + 1) = (\nu + 1)(\nu + 2). \quad (59.32c)$$

For the second the degeneracy is infinite.

Both of these possibilities were already discussed in Eqs. (59.12) and (59.13) and they are more clearly seen in Fig. XI.1. Thus it seems very useful to separate the two types of levels, as those associated with ϵ_ν and ϵ_n have respectively compact and noncompact symmetry Lie algebras.

For this purpose it is convenient to have projection operators that allow us to separate the states related with ϵ_ν from those corresponding to ϵ_n . To achieve this goal we note that the operator J^2 has eigenvalues $j(j+1)$, and thus the operator

$$\hat{J} \equiv (J^2 + \frac{1}{4})^{1/2} - \frac{1}{2} \quad (59.34a)$$

has eigenvalue j . The fact that there is a square root is irrelevant, if it is going to act on states of definite eigenvalue $j(j+1)$ of J^2 . In a similar manner we can define the operator

$$\hat{L} \equiv (L^2 + \frac{1}{4})^{1/2} - \frac{1}{2}. \quad (59.34b)$$

These two types of operators allow to define projection ones by

$$P^+ = \hat{L} - \hat{J} + \frac{1}{2}, \quad (59.35a)$$

$$P^- = \hat{J} - \hat{L} + \frac{1}{2}, \quad (59.35b)$$

as clearly P^+ when acting on a state where $\ell = j + 1/2$ gives 1, and 0 when $\ell = j - 1/2$, while correspondingly P^- gives 0 when $\ell = j + 1/2$ and 1 if $\ell = j - 1/2$.

If we apply P^+ to the states (59.4,9,17) we get only those corresponding to ϵ_ν , while when we apply P^- we get those of ϵ_n .

The degeneracy observed in (59.33c) for the states ϵ_ν suggests that it is due to an O(4) symmetry group and corresponds to its irreducible representation $[\nu + 1/2, 1/2]$ as it is well known that it will contain all the irreps $j = 1/2, 3/2 \dots, \nu + 1/2$ of the subgroup O(3), or, more correctly, of the SU(2) homomorphic to it.

The derivation of the six generators of o(4) Lie algebra, associated with the O(4) symmetry group, is a much more involved affair [6] than the corresponding one for unitary groups discussed in Chapter VII. We shall just state the result noting the o(3), or rather su(2), subalgebra of o(4) has obviously the three generators

$$J_q, \quad q = 1, 0, -1, \quad (59.36)$$

so we need to find three more that we shall designate by A_q , $q = 1, 0, -1$ and which take the values [6]

$$A_q = P^+ \frac{1}{4}[(\hat{J} + 2)^{-1}(H + 2\hat{J} + 2)^{1/2}F_q + H(J_q/J^2) + G_q(H + 2\hat{J} + 2)^{1/2}(\hat{J} + 2)^{-1}]P^+, \quad (59.37)$$

where \hat{J} , J^2 have already been defined, while

$$H = \boldsymbol{\eta} \cdot \boldsymbol{\xi} - 2\mathbf{L} \cdot \mathbf{S}, \quad (59.38a)$$

$$F_q = \eta_q(\boldsymbol{\eta} \cdot \boldsymbol{\xi} - \hat{L}) - (\boldsymbol{\eta} \cdot \boldsymbol{\eta})\xi_q, \quad (59.38b)$$

$$G_q = (-1)^q(F_{-q})^\dagger = (\boldsymbol{\eta} \cdot \boldsymbol{\xi} - \hat{L})\xi_q - \eta_q(\boldsymbol{\xi} \cdot \boldsymbol{\xi}), \quad (59.38c)$$

with $\boldsymbol{\eta}$, $\boldsymbol{\xi}$ given by (59.16) while η_q and ξ_q , $q = 1, 0, -1$, are their spherical components.

Turning now our attention to the states ϵ_n we note that, as they are infinitely degenerate, the symmetry group must be a noncompact one, and it turns out to be O(3,1) and its irrep is $[-1 + in, \frac{1}{2}]$ [6]. Of the six generators of o(3,1), three of them are the same J_q , $q = 1, 0, -1$, of (59.36), while the other three we designate as a_q , and they are given by

$$a_q = P^- \frac{1}{4}\{(\hat{J} - 1)^{-1}[(H^2 + 4\hat{J}^2)/(H + 2\hat{J})]^{1/2}f_q - H(J_q/J^2) + g_q[(H^2 + 4\hat{J}^2)/(H + 2\hat{J})]^{1/2}(\hat{J} - 1)^{-1}\}P^-, \quad (59.39)$$

where all symbols have been defined before except for f_q, g_q given by

$$f_q = \eta_q(\boldsymbol{\eta} \cdot \boldsymbol{\xi} + \hat{L} + 1) - (\boldsymbol{\eta} \cdot \boldsymbol{\eta})\xi_q, \quad (59.40a)$$

$$g_q = (-1)^q(f_{-q})^\dagger = (\boldsymbol{\eta} \cdot \boldsymbol{\xi} + \hat{L} + 1)\xi_q\eta_q(\boldsymbol{\xi} \cdot \boldsymbol{\xi}). \quad (59.40b)$$

The appearance of square roots and inverses of operators in (59.37), (59.39) and (59.38), (59.40), does not cause any problems, as they will be applied to wave functions (59.4,9,17) in which, $\boldsymbol{\eta} \cdot \boldsymbol{\xi}$, J^2 , \hat{J} , \hat{L} and $\mathbf{L} \cdot \mathbf{S}$ are diagonal, and thus become perfectly well defined numbers. In fact, it is the presence of the numerical matrix representation of the operators J_q and A_q on the states ϵ_ν , that allow us to identify them with the irrep $[\nu + 1/2, 1/2]$ of o(4) and, similarly, for the states ϵ_n we get the irrep $[-1 + in, \frac{1}{2}]$ of o(3,1).

For the full set of states of the type (59.4,9,17) we can then state that the symmetry Lie algebra is the direct sum

$$\text{so}(4) \oplus \text{so}(3, 1). \quad (59.41)$$

60 The Spinorial Relativistic Particle in an Electromagnetic Field

The problem with which we are going to deal here has been extensively discussed in the literature but as it gives rise, in part, to harmonic oscillator

states it is worthwhile analyzing it in the context of this book. Furthermore it will be generalized to a relativistic two particle problem with an interaction linear in the coordinates, but modulated by a constant antisymmetric tensor. This last problem, though not directly of physical interest, is worthwhile considering because its comparison with other types of two-body problems with Dirac oscillator interactions.

Thus we have the Lorentz invariant wave equation

$$[\gamma^\mu(p_\mu - \frac{e}{2}\epsilon_{\mu\nu\sigma\tau}x^\nu F^{\sigma\tau}) + 1]\psi = 0, \quad (60.1)$$

where γ^μ is given by (59.2,18) and x^μ, p_μ are four vectors of position and momentum, while $\epsilon_{\mu\nu\sigma\tau}$ is the four component completely antisymmetric tensor. The $F^{\sigma\tau}$ represents a constant antisymmetric tensor associated with an electromagnetic field, and e is the charge of the particle in the units we use in this Chapter.

We shall only consider a $F^{\sigma\tau}$ which, in an appropriate space time frame of reference, can be reduced to its purely magnetic part and thus we have in this frame

$$F^{ij} = 0 \quad ; \quad i, j = 1, 2, 3 \quad ; \quad F^{i0} = \frac{1}{2}\mathcal{H}^i, \quad (60.2)$$

so assuming a ψ of the form

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \exp(-iEx^0), \quad (60.3)$$

with ψ_1, ψ_2 , as before, being the large and small components of ψ , we get the equations

$$\sigma \cdot [\mathbf{p} - \frac{e}{2}(\mathbf{r} \times \mathcal{H})] \psi_2 = (E - 1)\psi_1, \quad (60.4)$$

$$\sigma \cdot [\mathbf{p} - \frac{e}{2}(\mathbf{r} \times \mathcal{H})] \psi_1 = (E + 1)\psi_2, \quad (60.5)$$

where \mathbf{r} is a vector of components (x_1, x_2, x_3) .

Multiplying (60.4) by $(E + 1)$ and substituting (60.5) we get for ψ_1 the equation

$$\begin{aligned} [(p_1^2 + p_2^2 + p_3^2) + \frac{e^2 \mathcal{H}^2}{4}(x_1^2 + x_2^2) + e\mathcal{H}(x_1 p_2 - x_2 p_1) + e\mathcal{H}\sigma_3] \psi_1 \\ = (E^2 - 1)\psi_1, \end{aligned} \quad (60.6)$$

where we took the coordinate x_3 in the direction of the magnetic field and expressed the vectors \mathbf{r}, \mathbf{p} in terms of their components.

The eigenvalues and eigenfunctions of equation (60.6) are well known [7] in terms of cylindrical coordinates, but we will rewrite it using creation

and annihilation operators, to obtain more directly the symmetry Lie algebra of this problem [11].

Let us define now the creation and annihilation operators in the plane x_1, x_2 as

$$\eta_i = \frac{1}{\sqrt{2}}[(\frac{e\mathcal{H}}{2})^{\frac{1}{2}}x_i - i(\frac{e\mathcal{H}}{2})^{-\frac{1}{2}}p_i], \quad \xi_i = \frac{1}{\sqrt{2}}[(\frac{e\mathcal{H}}{2})^{\frac{1}{2}}x_i + i(\frac{e\mathcal{H}}{2})^{-\frac{1}{2}}p_i], \quad (60.7)$$

with $i = 1, 2$. Furthermore we introduce the spherical components of these operators in the form

$$\eta^\pm = \frac{1}{\sqrt{2}}(\eta_1 \pm i\eta_2), \quad \xi^\pm = \frac{1}{\sqrt{2}}(\xi_1 \mp i\xi_2). \quad (60.8)$$

Equation (60.6) takes then the form

$$[e\mathcal{H}(2\eta_+ \xi^+ + 1) + p_3^2 + e\mathcal{H}\sigma_3]\psi_1 = (E^2 - 1)\psi_1. \quad (60.9)$$

The eigenfunctions of (60.9) can be written in the form of the ket

$$|n_+ n_- k\tau\rangle \equiv \frac{\eta_+^{n_+} \eta_-^{n_-} |0\rangle}{(n_+! n_-!)^{\frac{1}{2}}} \exp(ikx_3)\chi_\tau, \quad (60.10)$$

where

$$|0\rangle = \pi^{-\frac{1}{2}} \exp[-\frac{1}{2}(x_1^2 + x_2^2)] \quad (60.11)$$

is the ground state and n_\pm take the integer values $n_\pm = 0, 1, 2, \dots$. The χ_τ stands for the spin $\frac{1}{2}$ function with the projection $\tau = \pm\frac{1}{2}$.

The eigenvalue of the energy is then

$$E_{n_+ k\tau}^2 - 1 = e\mathcal{H}(2n_+ + 1 + 2\tau) + k^2, \quad (60.12)$$

and it does not depend on n_- . Thus there is an infinite degeneracy of the levels associated with the last quantum number and, as in fact the Hamiltonian in (60.9) commutes with $\eta_-, \xi^-, 1$, we have that the symmetry Lie algebra is given by the Weyl group of which they are the generators.

The Hamiltonian, in the form (60.6) or (60.9) commutes with the total angular momentum in the direction of the magnetic field, *i.e.*, with

$$x_1 p_2 - x_2 p_1 + \frac{1}{2}\sigma_3 = \eta_+ \xi^+ - \eta_- \xi^- + \frac{1}{2}\sigma_3. \quad (60.13)$$

The eigenvalue of this last operator can be denoted by

$$\mu = m + \tau, \quad (60.14)$$

where m is the orbital angular momentum in the direction of the field. It is then also convenient to characterize our state by the integrals of motion μ and n_- instead of n_+, n_- , as we have from (61.13) the relation

$$\mu = n_+ - n_- + \tau. \quad (60.15)$$

As p_3 is also an integral of motion, we can finally write our eigenfunction and eigenvalue as

$$|\mu nk\tau\rangle = \frac{\eta_+^{\mu+n-\tau} \eta_-^n |0\rangle}{[(\mu + n - \tau)! n!]^{1/2}} \exp(ikx_3) \chi_\tau, \quad (60.16)$$

$$E_{\mu n \kappa}^2 = 1 + 2e\mathcal{H}(\mu + n + \frac{1}{2}) + k^2, \quad (60.17)$$

where we have replaced n_- by just $n = 0, 1, 2, \dots$, while from (60.15) we see that μ is semiinteger either positive or negative.

The spectrum is continuous because k^2 is a real number in the interval $0 \leq k^2 \leq \infty$. Assuming though that the motion takes place exclusively in the plane perpendicular to the magnetic field, the spectrum is discrete and infinitely degenerate as for

$$\mu + n = \nu, \quad (60.18)$$

with ν being a fixed semiinteger, we can have the values

$$(\mu, n), (\mu \pm 1, n \mp 1), (\mu \pm 2, n \mp 2), \dots, \quad (60.19)$$

which stop when we reach $n = 0$ using the upper $-$ sign for n , but continues indefinitely when we use the lower $+$ sign.

The integrals of motion of the problem are, as we showed above, given by

$$\eta_-, \xi^-, p_3, \quad (60.20)$$

and thus the symmetry Lie algebra of this problem is given by the direct sum

$$w(1) \oplus t_3, \quad (60.21)$$

where the $w(1)$ is the Weyl algebra of generators $\eta_-, \xi^-, 1$, while t_3 is the translation algebra of generator p_3 .

If we wanted our solution (60.16), as well as our electromagnetic field $F^{\mu\nu}$ in (60.1) in another frame of reference, we would have to boost it following the same procedure as in section 59.

Finally we would like to stress that our Eq. (60.1), and more specifically its form (60.6), corresponds to the physical problem of an electron of spin 1/2 and charge e , in a constant magnetic field \mathcal{H} , of which many applications have been found.

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Chapter XII

The Two-Body Relativistic Oscillator

In the previous section we dealt with problems involving a one-body relativistic oscillator. Had we been considering ordinary quantum mechanics, the extension to n bodies would have been trivial, as Schroedinger himself was aware [1].

In the relativistic case though the situation is very different, even when dealing with two particles. In this section we will proceed to analyze the latter either through a single relativistic equation for the two-body system [2], or through two equations satisfying appropriate compatibility conditions [3,4]. The latter procedure will be reserved for the last section of this chapter, while for the former we start by discussing the system of two non-interacting spinorial particles. This system has been widely accepted in the literature, and already has some of the strange features that accompany the marriage of relativity and quantum mechanics.

61 The System of Two Non-Interacting Spinorial Particles and the Relativistic Cockroach Nest

In the units we are using, two free particles of spin 1/2 and equal mass are eigenstates of the sum of their corresponding Dirac Hamiltonians, *i.e.*,

$$(\alpha_1 \cdot p_1 + \beta_1 + \alpha_2 \cdot p_2 + \beta_2)\psi = E\psi, \quad (61.1)$$

where $\mathbf{p}_1, \mathbf{p}_2$ are the momenta of the two particles and, from (59.2), we have that

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \quad (61.2a)$$

$$\alpha_2 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \otimes \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \quad (61.2b)$$

$$\beta_1 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}, \quad (61.2c)$$

$$\beta_2 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \otimes \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad (61.2d)$$

where \otimes implies a direct product, and all the matrices appearing in (61.2) are of dimension 2×2 , with σ_1, σ_2 being the vector Pauli matrices of particles 1 and 2.

The reason we assert that (61.1) is the correct equation for the total energy E of the two particle system can be seen through the following considerations. First apply the operator on the left hand side of (61.1) to both sides of this equation and use the fact that α 's and β 's anticommute to get

$$\{[(p_1^2 + 1) + (p_2^2 + 1)] + 2(\alpha_1 \cdot \mathbf{p}_1 + \beta_1)(\alpha_2 \cdot \mathbf{p}_2 + \beta_2)\}\psi = E^2\psi. \quad (61.3)$$

Passing the square bracket of this last equation to the right hand side, and squaring the operators on both sides of the resulting equation we get finally

$$4(p_1^2 + 1)(p_2^2 + 1)\psi = [E^2 - (p_1^2 + 1) - (p_2^2 + 1)]^2\psi. \quad (61.4)$$

We can then assume for the solution of Eq. (61.4) the form

$$\exp[i(\mathbf{p}_1 \cdot \mathbf{x}_1 + \mathbf{p}_2 \cdot \mathbf{x}_2)], \quad (61.5)$$

with $\mathbf{p}_1, \mathbf{p}_2$ being now numerical three vectors, and we get for E the fourth degree equation

$$[E^2 - (p_1^2 + 1) - (p_2^2 + 1)]^2 - 4(p_1^2 + 1)(p_2^2 + 1) = 0, \quad (61.6)$$

whose four roots are easily seen to have the form

$$E = \pm(p_1^2 + 1)^{\frac{1}{2}} \pm (p_2^2 + 1)^{\frac{1}{2}}. \quad (61.7)$$

This is the result we expect classically from Einstein's relation $E^2 = p^2 + 1$ if the total energy is regarded as the sum of those of particles 1 and 2, *i.e.*, $E = E_1 + E_2$.

It is particularly interesting to consider the problem in the frame of reference in which the center of mass is at rest, *i.e.*, when

$$\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 = 0, \quad (61.8)$$

so we can write

$$\mathbf{p}_1 = -\mathbf{p}_2 \equiv \mathbf{p}, \quad (61.9)$$

in which case the total energy (61.7) can take the values

$$E = \begin{cases} (4p^2 + 4)^{\frac{1}{2}} \\ 0 \\ -(4p^2 + 4)^{\frac{1}{2}} \end{cases}. \quad (61.10)$$

There are positive and negative total energies above 2 and below -2, respectively, just as in the one-body problem, but a puzzling feature is the appearance of an energy $E = 0$ which, as we shall show below, implies an infinitely degenerate level in the relativistic quantum picture for two non-interacting particles. This level we shall denote as a *cockroach nest* [5], because it appears inert so long as the particles are free, but most interactions will bring out values at $E \neq 0$. The name we have given to this level comes from its analogy with a crack in a wall, which looks innocuous under normal circumstances, but if food is put near it, *i.e.*, in our case an interaction, the cockroaches start to come out. It is interesting to stress that our analogy indicates that if food is near the crack it will keep the cockroaches there, and thus will not hamper our use of the rest of the wall. We note though that food far from the crack will cause a veritable invasion of the whole wall. Similar results can be said to apply to our quantum problem when we pass from weak to strong interaction, *i.e.*, the levels coming out of $E = 0$ can mix with those of positive energy, and thus invalidate the use of the latter in a physically significant way.

We shall now proceed to discuss the solution of Eq. (61.1) in the center of mass frame to justify some of the statements of the previous paragraph.

a) The relativistic quantum problem for two non-interacting particles of spin 1/2

In the frame of reference where the center of mass is at rest, we see from (61.9) that Eq. (61.1) takes the form

$$[(\alpha_1 - \alpha_2) \cdot \mathbf{p} + \beta_1 + \beta_2]\psi = E\psi, \quad (61.11)$$

where $\alpha_1, \alpha_2, \beta_1, \beta_2$ are given by the direct products in (61.2) and thus can also be written as 4×4 matrices, for example

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_1 & 0 & 0 \\ \sigma_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sigma_1 \\ 0 & 0 & \sigma_1 & 0 \end{pmatrix}. \quad (61.12)$$

The wave function ψ in (61.11) can also be written as a direct product of two wave functions of the form (59.4) with large and small components and, in a way similar to the procedure followed for deriving (61.12), we can express ψ as a four-component vector

$$\psi = \begin{pmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{pmatrix}. \quad (61.13)$$

Thus Eq. (61.11) takes then the form

$$\begin{pmatrix} 0 & \sigma_1 \cdot p & -\sigma_2 \cdot p & 0 \\ \sigma_1 \cdot p & 0 & 0 & -\sigma_2 \cdot p \\ -\sigma_2 \cdot p & 0 & 0 & \sigma_1 \cdot p \\ 0 & -\sigma_2 \cdot p & \sigma_1 \cdot p & 0 \end{pmatrix} \begin{pmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{pmatrix} = \begin{pmatrix} (E-2)\psi_{11} \\ E\psi_{21} \\ E\psi_{12} \\ (E+2)\psi_{22} \end{pmatrix}. \quad (61.14)$$

Writing (61.14) explicitly, eliminating ψ_{21}, ψ_{12} between its terms to get an equation in ψ_{11}, ψ_{22} only, and finally defining the function ϕ_+, ϕ_- by the relation

$$\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{22} \end{bmatrix}, \quad (61.15)$$

we get the equation

$$\begin{bmatrix} 4(p \cdot S)^2 - E^2 & 2E \\ 2E & 4p^2 4(p \cdot S)^2 - E^2 \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = 0, \quad (61.16)$$

where

$$S = \frac{1}{2}(\sigma_1 + \sigma_2). \quad (61.17)$$

The matrix operator (61.16) commutes with

$$p^2, \quad J = L + S, \quad S^2, \quad (61.18)$$

so that they are integrals of motion, together with the parity as (61.16) remains invariant under inversion, i.e., $p \rightarrow -p$.

The eigenstates of (61.16) can then be characterized by the eigenvalues k^2 of p^2 , $j(j+1)$ of J^2 , m of J_3 , $s(s+1)$ of S^2 as well as the parity and thus can be expressed in terms of the kets

$$|k(\ell, s)jm\rangle = \sum_{\mu, \sigma} \sqrt{2j+1}(-1)^{\ell-s+m} \begin{pmatrix} \ell & s & j \\ \mu & \sigma & -m \end{pmatrix} \times j_\ell(kr) Y_{\ell\mu}(\theta, \varphi) \chi_{s\sigma}, \quad (61.19)$$

where (\cdot) is a $3j$ coefficient, $j_\ell(kr)$ the spherical Bessel function, $Y_{\ell\mu}(\theta, \varphi)$ the spherical harmonic and $\chi_{s\sigma}$ the spin function of the two particles with $s = 1$ or 0. The parity of the ket (61.19) is given by $(-1)^\ell$.

We note that for definite (k, j) and spin $s = 0$ we have the single state

$$|k(j, 0)jm\rangle, \quad (61.20)$$

whose parity $(-1)^j$. For spin $s = 1$ and parity $(-1)^j$ we also have a single state

$$|k(j, 1)jm\rangle, \quad (61.21)$$

while for parity $-(-1)^j$, we have two states:

$$|k(j \pm 1, 1)jm\rangle. \quad (61.22)$$

To get the eigenvalues E and eigenstates (ϕ_+, ϕ_-) of Eq. (61.16) we need to apply the operators appearing in the matrix to the states (61.19). This can be done using standard Racah algebra as was carried out in reference [5]. What is relevant for us is that in all the cases (61.20)–(61.22) we get a secular equation of the form

$$E^2(E^2 - 4k^2 - 4) = 0, \quad (61.23)$$

where k^2 is the eigenvalue of the relative square momentum p^2 , that appears in (61.18).

We proceed to derive explicitly the secular equation (61.23) for the case when $s = 0$, as all the others can be obtained similarly. From (61.20) we see that our states are then of the form

$$\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} a_+ \\ a_- \end{bmatrix} |k(j, 0)jm\rangle, \quad (61.24)$$

with the coefficients a_{\pm} depending only on k, j so that Eq. (61.16) becomes the numerical one

$$\begin{bmatrix} -E^2 & 2E \\ 2E & 4k^2 - E^2 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix} = 0, \quad (61.25)$$

which has a solution only if the determinant of the matrix vanishes, *i.e.*, if the energy satisfies the secular equation (61.23).

Clearly then besides the expected relation between energy and momentum $E^2 = 4k^2 + 4$ we have also the level $E = 0$ which we associated with the cockroach nest.

Introducing the roots $E = \pm(4k^2 + 4)^{\frac{1}{2}}$ in Eq. (61.25), we get the relation $a_- = (1/2)(4k^2 + 4)^{\frac{1}{2}} a_+$ and so we are left with the single constant a_+ . Using then (61.15) we can obtain ψ_{11}, ψ_{22} from ϕ_+, ϕ_- given by (61.24), and, in turn, we get from the second and third equation in (61.14) that ψ_{21}, ψ_{12} are proportional to operators of the form $\sigma_s \cdot p, s = 1, 2$ acting on ψ_{11}, ψ_{22} . The value of a_+ can then be determined by normalization.

The procedure of the previous paragraph unfortunately does not work for $E = 0$, where we must start directly from the matrix equation (61.14) in which we eliminate the E . Using then standard Racah algebra we can see straightforwardly that the states corresponding to parity $(-1)^j$, spin $s = 0$ and $E = 0$ can be written as

$$\psi_{11} = -\psi_{22} = -\sqrt{2k}[2(2j+1)]^{-\frac{1}{2}}[(j)^{\frac{1}{2}}b + (j+1)^{\frac{1}{2}}d] \times |k(j, 0)jm\rangle, \quad (61.26a)$$

$$\psi_{21} = \psi_{12} = -i[b|k(j-1, 1)jm\rangle + d|k(j+1, 1)jm\rangle], \quad (61.26b)$$

where we have two arbitrary constants b, d . Thus for $E = 0$ we obtain a double infinity of solutions for any k, j where the former is real and positive and the latter a nonnegative integer. The double character is due to the appearance of E^2 rather than E in the secular equation (61.23).

We have thus shown that for two free particles the energy $E = 0$, is also a possibility and corresponds to an infinitely degenerate state. We have taken the trouble to discuss it in this section because this level, to which we referred as a relativistic cockroach nest, appears in other problems where interactions are involved, and thus a clear understanding of it is required.

b) The Poincaré invariant equation for a system of non-interacting particles

Equation (61.1) for a system of two non-interacting particles does not have the Poincaré invariant form we obtained, for example, in the one-body

Klein-Gordon equation of Eq. (58.6) or the Dirac oscillator of Eqs. (59.19) or (59.21), but it can be put in this type of form with the help of the unit time like four vector $u_\mu, \mu = 0, 1, 2, 3$, of Eqs. (58.16) or (58.20). We shall proceed to show this, but for the more general problem of n free particles of spin $1/2$ and the same mass, so as to be able to use the result also in the next chapter.

We start then with the equation

$$\sum_{s=1}^n (\alpha_s \cdot p_s + \beta_s) \psi = E \psi, \quad (61.27)$$

where the matrices are direct products such as

$$\beta_s = I \otimes I \dots \otimes I \otimes \beta \otimes I \dots \otimes I, \quad (61.28)$$

with β in the position s , and similarly for the α_s .

As in the case of Eq. (59.18) for a single particle we can now have the four vector matrices γ_s^μ defined by

$$\gamma_s^0 = \beta_s, \quad (61.29a)$$

$$\gamma_s^i = \beta_s \alpha_{is}, \quad i = 1, 2, 3. \quad (61.29b)$$

With the help of the unit time like four vector u_μ of (58.20) we can define the Lorentz scalars

$$\Gamma \equiv \prod_{r=1}^n (\gamma_r^\mu u_\mu), \quad (61.30a)$$

$$\Gamma_s = (\gamma_s^\mu u_\mu)^{-1} \Gamma, \quad (61.30b)$$

where, as in the previous sections, repeated greek indices are summed over $\mu = 0, 1, 2, 3$. Note that $(\gamma_s^\mu u_\mu)^{-1}$ in (61.30b) just eliminates the corresponding term in Γ of (61.30a) so Γ_s is still in product form.

A procedure used by Barut [6] and his collaborators to derive variationally a single equation for an n -body system from a field theoretical action, suggested to us a Poincaré invariant equation of the form

$$\left[\sum_{s=1}^n \Gamma_s (\gamma_s^\mu p_{\mu s} + 1) \right] \psi = 0 \quad (61.31)$$

for the system of n free particles of spin $1/2$.

We proceed now to show that Eq. (61.31) reduces to Eq. (61.27) when (u_μ) takes its values (58.16), *i.e.*, $(u_\mu) = (1, 0, 0, 0)$. In that case Eq. (61.31) takes the form

$$\left[\Gamma^0 \sum_{s=1}^n p_{0s} + \sum_{s=1}^n \Gamma_s^0 (\gamma_s \cdot \mathbf{p}_s + 1) \right] \psi = 0, \quad (61.32)$$

with

$$\Gamma^0 \equiv \prod_{r=1}^n \gamma_r^0, \quad (61.33a)$$

$$\Gamma_s^0 \equiv (\gamma_s^0)^{-1} \Gamma^0, \quad (61.33b)$$

and where boldface letters mean ordinary three-dimensional vectors.

Multiplying (61.32) by Γ^0 , and making use of (61.29) and (59.2) and that $(\gamma_s^0)^{-1}$ is also β_s , we obtain

$$\left[-P^0 + \sum_{s=1}^n (\alpha_s \cdot \mathbf{p}_s + \beta_s) \right] \psi = 0, \quad (61.34)$$

where we denote by $P_\mu, \mu = 0, 1, 2, 3$ the total four momentum four vector

$$P_\mu = \sum_{s=1}^n p_{\mu s}, \quad (61.35)$$

of which P_0 is its time-like component and, in our metric (58.3), equals $-P_0$. As P^0 is then the total energy E of the system we recovered Eq. (61.27).

Thus we have in (61.31) the Poincaré invariant form of the equation for a system of n free particles.

With this achievement we leave the discussion of the free particle problem and turn our attention to systems in which there is an oscillator interaction.

62 The Two-Body System with a Dirac Oscillator Interaction

In section 59, where the Dirac oscillator concept was introduced, it was sufficient to replace in the free particle Dirac equation the momentum \mathbf{p} by $\mathbf{p} - i\omega \mathbf{r}\beta$, where \mathbf{r} was the coordinate canonically conjugate to \mathbf{p} .

For a two-body system, with an interaction depending on the relative coordinates between them our interest will initially be confined to the frame of reference where the center of mass is at rest, as the total momentum four vector $P_\mu, \mu = 0, 1, 2, 3$, of (61.35) will continue to be an integral of motion and, in the frame mentioned, $P_i = 0, i = 1, 2, 3$ while $P_0 = -P^0$, where the latter is the total energy of the system, i.e., $P^0 = E$.

Thus a two-body system with a Dirac oscillator interaction will satisfy an equation of the type (61.11) if we replace in it

$$\mathbf{p} \rightarrow \mathbf{p} - i(\omega/2)\mathbf{r}B, \quad (62.1)$$

where

$$\mathbf{p} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2), \quad \mathbf{r} = (\mathbf{x}_1 - \mathbf{x}_2), \quad (62.2)$$

while B is a matrix that has to be determined in such a way that some form of oscillator interaction appears, and the problem has an explicitly analytic solution. The factor (1/2) in the frequency appearing in (62.1) was introduced for convenience when we later discuss the nonrelativistic limit of our equations.

To begin with we note that in the one-body problem (59.3) we had a β instead of a B , which anticommuted with the α , and this was fundamental for the reduction of the problem to Eq. (59.6) where the oscillator appeared explicitly together with a strong spin-orbit coupling term.

In the present case, if we make the substitution (62.1) in (61.11), we would like the matrix B to anticommute both with α_1 and α_2 and this is a strong restriction on B . Actually two possibilities are suggested immediately for a B with the properties mentioned above which are the following:

$$B = \beta_1 \beta_2, \quad (62.3a)$$

and

$$B = \beta_1 \beta_2 \gamma_{51} \gamma_{52}, \quad (62.3b)$$

where

$$\gamma_{5s} = i\gamma_s^0 \gamma_s^1 \gamma_s^2 \gamma_s^3, \quad s = 1, 2, \quad (62.3c)$$

is a pseudo-scalar matrix usually denoted by that name in the literature [7]. It is clear then that $\gamma_{51} \gamma_{52}$ is a Lorentz scalar.

The equation, in the frame of reference where the center of mass is at rest, for the two-body system with a Dirac oscillator type of interaction can then be written as

$$\{(\alpha_1 - \alpha_2) \cdot [\mathbf{p} - i(\omega/2)\mathbf{r}B] + \beta_1 + \beta_2\} \psi = E\psi, \quad (62.4)$$

where B can have either the form (3a) or (3b).

As in the case of the one-body system, in section 59, we proceed first to solve Eq. (62.4), before proving afterwards that it can be put in a Lorentz invariant form, and outlining later the algebras responsible for the degeneracies.

a) Solution of Eq. (62.4) when $B = \beta_1\beta_2$

If we write $\alpha_1, \alpha_2, \beta_1\beta_2$ in the (4×4) matrix form indicated in (61.12), and denote the wave function in the four-component vector form (61.13) we obtain, when $B = \beta_1\beta_2$ that Eq. (62.4) takes the form

$$\begin{bmatrix} 2 & \sigma_1 \cdot [p + i\frac{1}{2}\omega r] & -\sigma_2 \cdot [p + i\frac{1}{2}\omega r] & 0 \\ \sigma_1 \cdot [p - i\frac{1}{2}\omega r] & 0 & 0 & -\sigma_2 \cdot [p - i\frac{1}{2}\omega r] \\ -\sigma_2 \cdot [p - i\frac{1}{2}\omega r] & 0 & 0 & \sigma_1 \cdot [p - i\frac{1}{2}\omega r] \\ 0 & -\sigma_2 \cdot [p + i\frac{1}{2}\omega r] & \sigma_1 \cdot [p + i\frac{1}{2}\omega r] & -2 \end{bmatrix} \times \begin{bmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{bmatrix} = E \begin{bmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{bmatrix}. \quad (62.5)$$

Introducing now the creation and annihilation operators by the definition

$$\eta = (1/\sqrt{2})[(\omega/2)^{\frac{1}{2}}r - i(\omega/2)^{-\frac{1}{2}}p], \quad (62.6a)$$

$$\xi = (1/\sqrt{2})[(\omega/2)^{\frac{1}{2}}r + i(\omega/2)^{-\frac{1}{2}}p], \quad (62.6b)$$

which imply that

$$p + i(\omega/2)r = i\sqrt{\omega}\eta, \quad (62.7a)$$

$$p - i(\omega/2)r = -i\sqrt{\omega}\xi, \quad (62.7b)$$

we see that Eq. (62.5) reduces to the form

$$i\sqrt{\omega} \begin{bmatrix} \sigma_1 \cdot \eta & -\sigma_2 \cdot \eta \\ -\sigma_2 \cdot \eta & \sigma_1 \cdot \eta \end{bmatrix} \begin{bmatrix} \psi_{21} \\ \psi_{12} \end{bmatrix} = \begin{bmatrix} E - 2 & 0 \\ 0 & E + 2 \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{22} \end{bmatrix}, \quad (62.8a)$$

$$-i\sqrt{\omega} \begin{bmatrix} \sigma_1 \cdot \xi & -\sigma_2 \cdot \xi \\ -\sigma_2 \cdot \xi & \sigma_1 \cdot \xi \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{22} \end{bmatrix} = E \begin{bmatrix} \psi_{21} \\ \psi_{12} \end{bmatrix}. \quad (62.8b)$$

Multiplying Eq. (62.8a) by E , introducing in it (62.8b), and finally passing from the functions ψ_{11}, ψ_{22} to the functions ϕ_+, ϕ_- through the relation (61.15), we obtain the matrix operator equation

$$O \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} 4\omega(\eta \cdot S)(\xi \cdot S) - E^2 & 2E \\ 2E & 4\omega[\eta \cdot \xi - L \cdot S - (\eta \cdot S)(\xi \cdot S)] - E^2 \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = 0, \quad (62.9)$$

where, as before, we have

$$S = \frac{1}{2}(\sigma_1 + \sigma_2), \quad (62.10a)$$

$$L = -i(\eta \times \xi). \quad (62.10b)$$

Clearly the matrix operator O commutes with

$$\hat{N} \equiv \eta \cdot \xi, \quad (62.11a)$$

$$J = L + S, \quad (62.11b)$$

$$S^2, \quad (62.11c)$$

as well as with the parity P as O remains invariant under inversion, *i.e.*, when

$$\eta \rightarrow -\eta, \quad \xi \rightarrow -\xi. \quad (62.12)$$

The states can then be characterized by the eigenvalues of

$$\hat{N}, J^2, J_3, S^2, P, \quad (62.13)$$

which are operators that commute among themselves, and that can be denoted respectively as

$$N, j(j+1), \quad m, \quad s(s+1), \quad \pm. \quad (62.14)$$

As $\omega[\hat{N} + (3/2)]$ is the Hamiltonian of a three-dimensional oscillator of frequency ω , we can express ϕ_{\pm} in terms of the ket similar to those of (59.9), but where now the spin takes the values $s = 0$ or 1 so the corresponding χ functions are

$$\chi_{s\sigma}; \quad s = 0, \quad \sigma = 0; \quad s = 1, \quad \sigma = 1, 0, -1. \quad (62.15)$$

Thus ϕ_{\pm} can be given in terms of the kets

$$|N(\ell, s)jm\rangle = \sum_{\mu, \sigma} \sqrt{2j+1}(-1)^{\ell-s+m} \begin{pmatrix} \ell & s & j \\ \mu & \sigma & -m \end{pmatrix} R_{N\ell}(\sqrt{\omega/2}r) Y_{\ell\mu}(\theta, \varphi) \chi_{s\sigma}, \quad (62.16)$$

with the same meaning for all the functions and symbols as in Eq. (59.9), and parity is given by $(-1)^{\ell}$.

We note that for definite (N, j) and spin $s = 0$ the parity is $(-1)^j$ and we have the single state

$$|N(j, 0)jm\rangle. \quad (62.17)$$

For spin $s = 1$ and parity $(-1)^j$ we also have the single state

$$|N(j, 1)jm\rangle, \quad (62.18)$$

while for parity $-(-1)^j$ we have the two states

$$|N(j \pm 1, 1)jm\rangle. \quad (62.19)$$

The calculation of the eigenvalues E in Eq. (62.9) involves then three separate problems according to the situations indicated above.

If $s = 0$, the solution is simple, *i.e.*, given by

$$\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} a_+ \\ a_- \end{bmatrix} |N(j, 0)jm\rangle, \quad (62.20)$$

where a_{\pm} are constants depending only on N, j . Applying the operator O of (62.9) to (ϕ_+, ϕ_-) of (62.20) we get the numerical equation

$$\begin{bmatrix} -E^2 & 2E \\ 2E & 4\omega N - E^2 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix} = 0, \quad (62.21)$$

as for a state of spin 0 the term $(S \cdot \eta)(S \cdot \xi)$ vanishes. Thus a solution exists only if the determinant of the matrix vanishes which gives the secular equation

$$E^2(E^2 - 4 - 4\omega N) = 0. \quad (62.22)$$

For the state of spin $s = 0$ of (62.17) we have then the eigenvalues

$$E^2 = 0, \quad (62.23a)$$

$$E_N^2 = 4 + 4\omega N. \quad (62.23b)$$

The first $E^2 = 0$ corresponds to states in the cockroach nest already discussed in the previous section. For the second, *i.e.*, $E_N^2 = 4 + 4\omega N$ we have an equally spaced spectrum for the square of the energy. From Eq. (62.21) we see also that the normalized a_{\pm} are given by

$$a_+ = (2 + \omega N)^{-\frac{1}{2}}, \quad (62.24a)$$

$$a_- = (1 + \omega N)^{\frac{1}{2}}(2 + \omega N)^{-\frac{1}{2}}. \quad (62.24b)$$

The wave functions $\psi_{st}, s, t = 1, 2$ associated with these values of ϕ_+ and ϕ_- can be obtained by procedures similar to those outlined after Eq. (61.25) for the case of two free particles.

Turning now our attention to the states (62.18,19) where the spin is 1, we see that the situation is more complex because we need the matrix elements of $(S \cdot \eta), (S \cdot \xi)$ with respect to those states, and from them we can calculate the matrix representation of $(S \cdot \eta), (S \cdot \xi)$ in those basis.

For the case of spin $s = 1$ but parity $(-1)^j$ we can obtain by straightforward Racah algebra [8] that

$$\begin{aligned} \langle N(j, 1)jm | \eta \cdot S | N - 1(j + 1, 1)jm \rangle \\ = [(N - j)j / (2j + 1)]^{\frac{1}{2}}, \end{aligned} \quad (62.25a)$$

$$\begin{aligned} \langle N(j, 1)jm | \eta \cdot S | N - 1(j - 1, 1)jm \rangle \\ = -[(N + j + 1)(j + 1) / (2j + 1)]^{\frac{1}{2}}, \end{aligned} \quad (62.25b)$$

and the corresponding matrices $(\xi \cdot S)$ can be determined by Hermitian conjugation. Thus for the case (62.18) we have

$$\langle N(j, 1)jm | \omega(\eta \cdot S)(\xi \cdot S) | N(j, 1)jm \rangle = \omega(N + 1). \quad (62.26)$$

We can then propose a solution of Eq. (62.9) in the form

$$\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} b_+ \\ b_- \end{bmatrix} |N(j, 1)jm\rangle, \quad (62.27)$$

with b_{\pm} being constants function of N, j , and from (62.26) this leads to the matrix equation

$$\begin{bmatrix} 4\omega(N + 1) - E^2 & 2E \\ 2E & -E^2 \end{bmatrix} \begin{bmatrix} b_+ \\ b_- \end{bmatrix} = 0, \quad (62.28)$$

which has a solution only when the secular equation

$$E^2[E^2 - 4 - 4\omega(N + 1)] = 0 \quad (62.29)$$

is satisfied.

For the state of spin $s = 1$ and parity $(-1)^j$ of (62.18) we have then the eigenvalues

$$E^2 = 0, \quad (62.30a)$$

$$E_N^2 = 4 + 4\omega(N + 1). \quad (62.30b)$$

The $E^2 = 0$ corresponds to states in the cockroach nest already discussed in the previous section. For $E_N^2 = 4 + 4\omega(N + 1)$ we have an equally spaced spectrum for the square of the energy but displaced by one quantum from

the value when the spin is $s = 0$. From Eq. (62.28) we also see that the normalized b_{\pm} are given by

$$\begin{aligned} b_+ &= \{[1 + \omega(N + 1)]/[2 + \omega(N + 1)]\}^{\frac{1}{2}}, \\ b_- &= [2 + \omega(N + 1)]^{-\frac{1}{2}}. \end{aligned} \quad (62.31)$$

For $s = 1$ and parity $(-1)^j$ the wave functions $\psi_{st}, s, t = 1, 2$ associated with these values of (ϕ_+, ϕ_-) can be obtained by procedures similar to those outlined for the case $s = 0$.

Turning now our attention to the case of spin $s = 1$ but parity $-(-1)^j$ of (62.19) we see that we require the following matrix elements

$$\begin{aligned} \langle N(j+1, 1)jm | \sqrt{\omega} \mathbf{S} \cdot \boldsymbol{\eta} | N-1(j, 1)jm \rangle \\ = -\sqrt{\omega} [j(N+j+2)/(2j+1)]^{\frac{1}{2}} \equiv (a/2), \end{aligned} \quad (62.32a)$$

$$\begin{aligned} \langle N(j-1, 1)jm | \sqrt{\omega} \mathbf{S} \cdot \boldsymbol{\eta} | N-1(j, 1)jm \rangle \\ = \sqrt{\omega} [(j+1)(N-j+1)/(2j+1)]^{\frac{1}{2}} \equiv (b/2), \end{aligned} \quad (62.32b)$$

which again are obtained by straightforward Racah algebra [8], while the matrix elements of $(\xi \cdot \mathbf{S})$ can be obtained from those of $(\eta \cdot \mathbf{S})$ in (62.32) by hermitian conjugation.

We can now propose a solution of Eq. (62.9) of the form

$$\begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} c_{++} \\ c_{--} \end{bmatrix} |N(j+1, 1)jm\rangle + \begin{bmatrix} c_{+-} \\ c_{-+} \end{bmatrix} |N(j-1, 1)jm\rangle, \quad (62.33)$$

where again $c_{\pm\pm}$ are constants functions of N, j , and from (62.32) this leads to the numerical matrix equation

$$\begin{bmatrix} a^2 - E^2 & -ab & 2E & 0 \\ -ab & b^2 - E^2 & 0 & 2E \\ 2E & 0 & a^2[(j+1)/j] - E^2 & ab \\ 0 & 2E & ab & b^2[j/(j+1)] - E^2 \end{bmatrix} \times \begin{bmatrix} c_{++} \\ c_{+-} \\ c_{-+} \\ c_{--} \end{bmatrix} = 0, \quad (62.34)$$

which has a solution only for those values of E for which the determinant of the matrix vanishes.

Substituting in the matrix (62.34) the values of a, b given in (62.32) we arrive at the secular equation

$$\begin{aligned} E^2 \{ E^2[E^2 - 4 - 4\omega(N+1)][E^2 - 4 - 4\omega(N+2)] \\ - 64\omega^2 j(j+1) \} = 0. \end{aligned} \quad (62.35)$$

One of the roots $E^2 = 0$ is independent of the values N, j and thus is associated with the cockroach nest discussed in the previous section. The other three roots of the square of the energy are given by a solution of a cubic equation in this variable. If $\omega \ll 1$ it is clear that two of the roots E^2 will be close to 4, while another is close to 0. The latter implies that cockroaches, i.e., energy levels, have come out of the nest due to the interaction just as we predicted in the previous section. The interesting levels are those of E^2 when it is close to 4, or $E \approx 2$ which, in our units, is the mass of the two particles. For those levels the normalized $c_{\pm\pm}$ where obtained in Appendix A of reference [9] and thus the (ϕ_+, ϕ_-) of (62.33) are known explicitly. The corresponding $\psi_{st}, s, t = 1, 2$ can be derived by procedures similar to those indicated for the case $s = 0$.

We have thus arrived at a complete solution for the energy eigenvalues and their corresponding wave functions of Eq. (62.4) when $B = \beta_1 \beta_2$. We shall proceed now to discuss the other case indicated in Eq. (62.3b).

b) Solution of Eq. (62.4) when $B = \beta_1 \beta_2 \gamma_{51} \gamma_{52}$

If we again write $\alpha_1, \alpha_2, \beta_1, \beta_2$ in the (4×4) matrix form indicated in (61.12) and denote the ψ in the four-component vector form (61.13), and finally introduce the definitions

$$a_{\pm} \equiv (\sigma_1 \cdot \mathbf{p}) \pm i(\omega/2)(\sigma_2 \cdot \mathbf{r}), \quad (62.36a)$$

$$b_{\pm} \equiv -(\sigma_2 \cdot \mathbf{p}) \pm i(\omega/2)(\sigma_1 \cdot \mathbf{r}), \quad (62.36b)$$

we see that Eq. (62.4), when $B = \beta_1 \beta_2 \gamma_{51} \gamma_{52}$, becomes

$$\begin{bmatrix} 2 & a_- & b_+ & 0 \\ a_+ & 0 & 0 & b_- \\ b_- & 0 & 0 & a_+ \\ 0 & b_+ & a_- & -2 \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{bmatrix} = E \begin{bmatrix} \psi_{11} \\ \psi_{21} \\ \psi_{12} \\ \psi_{22} \end{bmatrix}. \quad (62.37)$$

Following then exactly the same procedure that allows us to go from (62.5) to (62.9) we arrive at the equation

$$\begin{bmatrix} A - E^2 & 2E \\ 2E & D - E^2 \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = 0, \quad (62.38)$$

where

$$A \equiv (a_- - b_+)(a_+ - b_-)$$

$$= 4\omega[S^2 + (\mathbf{S} \cdot \boldsymbol{\eta})(\mathbf{S} \cdot \boldsymbol{\xi}) + \mathbf{L} \cdot \mathbf{S}], \quad (62.39a)$$

$$D \equiv (a_- + b_+)(a_+ + b_-) \quad (62.39b)$$

$$= 4\omega[\hat{N} - (\mathbf{S} \cdot \boldsymbol{\eta})(\mathbf{S} \cdot \boldsymbol{\xi}) - \mathbf{L} \cdot \mathbf{S}], \quad (62.39b)$$

with $\boldsymbol{\eta}, \boldsymbol{\xi}$ given in (62.6) and \mathbf{L}, \mathbf{S} by (62.10).

The eigenvalues and eigenstates of Eq. (62.38) can be derived by the same procedure followed in the case of (62.9). We have again three cases, $s = 0$, parity $(-1)^j$ of (62.17); $s = 1$, parity $(-1)^j$ of (62.18); and $s = 1$, parity $-(-1)^j$ of (62.19). We require the matrix elements (62.25,32) and of their hermitian conjugates, plus the fact that

$$\mathbf{L} \cdot \mathbf{S} = (1/2)(J^2 - L^2 - S^2). \quad (62.40)$$

Thus for $s = 0$ we take (ϕ_+, ϕ_-) in the form (62.20) and arrive at the numerical matrix equation

$$\begin{bmatrix} -E^2 & 2E \\ 2E & 4\omega N - E^2 \end{bmatrix} \begin{bmatrix} a_+ \\ a_- \end{bmatrix} = 0, \quad (62.41)$$

which leads to the secular equation

$$E^2(E^2 - 4 - 4\omega N) = 0 \quad (62.42)$$

with the same roots:

$$E^2 = 0, \quad (62.43a)$$

$$E_N^2 = 4 + 4\omega N, \quad (62.43b)$$

as in the case when $B = \beta_1\beta_2$ and the same interpretation.

For $s = 1$, parity $(-1)^j$ we take (ϕ_+, ϕ_-) in the form (62.27) and using the matrix element (62.26) arrive at the numerical matrix equation

$$\begin{bmatrix} 4\omega(N+2) - E^2 & 2E \\ 2E & -E^2 \end{bmatrix} \begin{bmatrix} b_+ \\ b_- \end{bmatrix} = 0, \quad (62.44a)$$

which leads to the secular equation

$$E^2[E^2 - 4 - 4\omega(N+2)] = 0, \quad (62.44b)$$

whose roots are

$$E^2 = 0, \quad (62.45a)$$

$$E_N^2 = 4 + 4\omega(N+2), \quad (62.45b)$$

where we note that E_N^2 in this case differs from the situation when $B = \beta_1\beta_2$, where it had the form (62.30b). The interpretation of the roots in Eq. (62.45) is though the same as in Eq. (62.30).

Finally for $s = 1$, parity $-(-1)^j$ we take (ϕ_+, ϕ_-) in the form (62.33) and arrive at the numerical matrix equation

$$\begin{bmatrix} \alpha^2 - E^2 & -\alpha\beta & 2E & 0 \\ -\alpha\beta & \beta^2 - E^2 & 0 & 2E \\ 2E & 0 & \beta^2 - E^2 & \alpha\beta \\ 0 & 2E & \alpha\beta & \alpha^2 - E^2 \end{bmatrix} \begin{bmatrix} c_{++} \\ c_{+-} \\ c_{-+} \\ c_{--} \end{bmatrix} = 0, \quad (62.46)$$

where

$$\alpha \equiv 2\sqrt{\omega}[j(N-j+1)/(2j+1)]^{1/2}, \quad (62.47a)$$

$$\beta \equiv 2\sqrt{\omega}[(j+1)(N+j+2)/(2j+1)]^{1/2}, \quad (62.47b)$$

and it leads to the secular equation

$$E^4[E^2 - (\alpha^2 + \beta^2 + 4)]^2 = 0, \quad (62.48)$$

so that using (62.47) we have the double roots

$$E^2 = 0, \quad (62.49a)$$

$$E_N^2 = 4 + 4\omega(N+2). \quad (62.49b)$$

Again $E^2 = 0$ is associated with an infinitely degenerate state in the cockroach nest, while we now have $E_N^2 = 4 + 4\omega(N+2)$ for spin $s = 1$, independently of the parity and it gives equal spacing for the square of the energy. This problem has extraordinary accidental degeneracy which we will discuss later on.

Thus we have achieved the complete solution of Eq. (62.4) both when $B = \beta_1\beta_2$ and when $B = \beta_1\beta_2\gamma_{51}\gamma_{52}$.

c) Poincaré invariant form of the two particle system with a Dirac oscillator interaction

Equation (62.4) has a perfectly definite form in the frame of reference where the center of mass is at rest. We would like though to express it as a Poincaré invariant equation for a two particle system with interaction.

We achieved this for the system of n -free particles, with the help of the unit time like four vector (u_μ) , as seen in Eq. (61.31). It is now just a question of particularizing this equation to $n = 2$ particles, and also to introduce in it the Dirac oscillator interaction. For the latter purpose it is

convenient to consider the coordinate four vectors $x_{\mu s}, \mu = 0, 1, 2, 3; s = 1, 2$, of the two particles and introduce again their transversal part as in (58.17), *i.e.*,

$$x_{\perp \mu s} = x_{\mu s} + (x_{\nu s} u^{\nu}) u_{\mu}. \quad (62.50)$$

We cannot replace $p_{\mu s}$ in (61.31) by a linear combination of it with $x_{\perp \mu s}$, with appropriate matrix coefficients, as we did in the one particle problem of (59.19), because $x_{\perp \mu s}$ is not translationally invariant. We can though overcome this obstacle by considering the coordinate four vectors with respect to the center of mass, *i.e.*,

$$x'_{\mu s} = x_{\mu s} - X_{\mu}, \quad (62.51a)$$

$$X_{\mu} = (1/2)(x_{\mu 1} + x_{\mu 2}), \quad (62.51b)$$

and take the transverse part of latter $x'_{\perp \mu s}$ defined as in (62.50). With these coordinates we can write down a Poincaré invariant equation for a two particle system with a Dirac oscillator interaction, of the form

$$\left\{ \sum_{s=1}^2 \Gamma_s [\gamma_s^{\mu} (p_{\mu s} - i\omega x'_{\perp \mu s} \Gamma) + 1] \right\} \psi = 0, \quad (62.52)$$

where Γ, Γ_s are defined as in (61.30).

Equation (62.52) has in it the unit time like four vector (u_{μ}) and we would like this vector to take its form (u_{μ}) = (1, 0, 0, 0) in the frame of reference where the center of mass is at rest. This is easily achieved by defining (u_{μ}) as

$$u_{\mu} \equiv P_{\mu} (-P_{\tau} P^{\tau})^{-\frac{1}{2}}, \quad (62.53)$$

where P_{μ} is the total four vector momentum (61.35). Thus in the center of mass frame as $P_i = 0, i = 1, 2, 3$ and $P_0 = -P^0$, we have that (u_{μ}) = (1, 0, 0, 0), and in this frame

$$\Gamma \rightarrow \Gamma^0 = \gamma_1^0 \gamma_2^0, \quad (62.54a)$$

$$\Gamma_1 \rightarrow \Gamma_1^0 = \gamma_2^0, \quad (62.54b)$$

$$\Gamma_2 \rightarrow \Gamma_2^0 = \gamma_1^0, \quad (62.54c)$$

as indicated in (61.33). Thus when multiplying by Γ^0 the resulting equation (62.52) in this frame of reference we get, in a similar way as in the case of (61.34), that the equation becomes

$$\{-P^0 + (\alpha_1 - \alpha_2) \cdot [p - i(\omega/2)r\beta_1\beta_2] + \beta_1 + \beta_2\} \psi = 0, \quad (62.55)$$

where in the center of the mass frame $p_1 = -p_2 \equiv p$ and $r = (x_1 - x_2)$.

Equation (62.55) is identical to (62.4), when $B = \beta_1\beta_2$ if we interpret P^0 , as is usually done, as the total energy E . Thus we have in (62.52) a Poincaré invariant equation for the two-body system with harmonic oscillator interaction for the case (62.3a). For (62.3b) we just have to replace Γ by $\Gamma\gamma_1\gamma_2$ and the latter continues to remain Poincaré invariant as we noted before that $\gamma_1\gamma_2$ is a scalar.

We have obtained in the previous pages the eigenfunctions of the problem (62.4) in the frame of reference where the center of mass is at rest, and to get those of (62.55) we just have to add the factor $\exp(-iEX^0)$, where X^0 is the time-like component of the center of mass coordinate four vector in (62.51b). If we wish to get the wave function in any other frame of reference, we have to boost both the relative and center of mass coordinates as in (58.24), and furthermore apply a direct product of two spinorial matrices \mathcal{U} of (59.32) in which the σ is replaced by σ_1 and σ_2 . A detailed discussion of this point is given in reference [9].

d) Symmetry algebras and superalgebras of the two-body system with Dirac oscillator interaction

When discussing Eq. (62.4) when $B = \beta_1\beta_2$ we noticed in (62.23b) and (62.30b) that there is accidental degeneracy for E_N^2 when $s = 0$ or $s = 1$ but with parity $(-1)^j$, as in these cases $\ell = j$ and for a given N we have

$$j = N, N-2, \dots, 1 \quad \text{or} \quad 0. \quad (62.56)$$

There is no accidental degeneracy when the parity is $-(-1)^j$ as the roots are given by the third degree algebraic equation, involving both N and j , in the curly bracket of (62.35). Thus we need to concentrate only of the states with parity $(-1)^j$, whose accidental degeneracy we wish to explain by a symmetry Lie algebra.

We start by drawing the levels, and noticing first that the state $N = 0, j = 0, s = 1$ cannot exist as $\ell = j = 0$ and the addition of angular momenta 0 and 1 cannot give a total of 0. We introduce then the symbol

$$\nu \equiv (4\omega)^{-1}(E_N^2 - 4) = N + s, \quad (62.57)$$

which, from (62.23b,30b), would apply to both the $s = 0$ and $s = 1$ situation when the parity is $(-1)^j$.

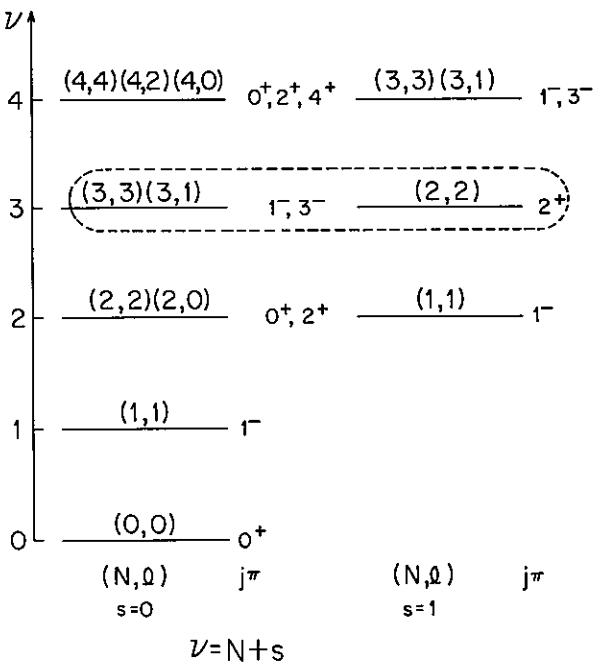


Figure XII.1. Levels of the spectra (62.58) of the relativistic problem for the cases when $s = 0$ and $s = 1$, where in both $j = \ell$. The dashed line surrounds an example of the kind of degeneracy we want to explain.

In Fig. XII.1, we draw the levels where the ordinate is the ν defined in (62.57), and on the right hand side of each level are the values of the total angular momentum j which equals the orbital one ℓ , so the parity $(-1)^j$ is also indicated as an upper \pm index on j . Above the level the values or (N, ℓ) are also given.

For spin $s = 0$ the levels start with $N = 0$, i.e., $\nu = 0$, but for spin $s = 1$, the ket $|0(0, 1)0\rangle$ does not exist so we start with $N = 1$ and $\nu = 2$. We surround by a dotted curve a level with the type of degeneracy we want to explain.

It is clear from the figure that for even ν we have the values of j and parity of the form

$$j^\pi = 0^+, 1^-, 2^+, 3^-, \dots, (\nu - 1)^-, \nu^+, \quad (62.58a)$$

while for ν odd, they become

$$j^\pi = 1^-, 2^+, 3^-, \dots, (\nu - 1)^+, \nu^-. \quad (62.58b)$$

62. THE TWO-BODY SYSTEM

Purely a dimensionality argument, as in a) of section 59, suggests that for even ν we are dealing with the irrep $[\nu, 0]$ of $O(4)$ group, while for odd ν the irrep is $[\nu, 1]$. This conclusion is also supported by the fact the subgroup $O(3)$ of $O(4)$, has the irreps j^π given in (62.58).

Of the six generators of the $o(4)$ Lie algebra, three are the components of the total angular momentum J_q , $q = 1, 0, -1$, while the other three, which can be denoted by A_q , $q = 1, 0, -1$ can be derived by a procedure similar to the one outlined in a) of section 59. A full analysis of the problem is given in reference [10].

A more interesting situation occurs when in Eq. (62.4) we use a B of the type $B = \beta_1\beta_2\gamma_{51}\gamma_{52}$ as then in all cases E_N is given by

$$E_N^2 = 4 + 4\omega[N + s(s + 1)], s = 0, 1, \quad (62.59)$$

as seen in Eqs. (62.43b, 45b, 49b). Again we have accidental degeneracy as $\ell = N, N - 2, \dots, 0$ or 1, but we have to be careful to distinguish cases when the parity is $(-1)^j$ and $\ell = j$, and those when it is $-(-1)^j$ and $\ell = j \pm 1$.

The explanation of the degeneracy (62.59) is best expressed in terms of a superalgebra, which requires that we not only consider the equation (62.4) with $B = \beta_1\beta_2\gamma_{51}\gamma_{52}$ and given ω , but also its super partner [11] where in (62.4) ω is replaced by $-\omega$. The analysis of the latter problem is then entirely similar to the one carried out between Eqs. (62.37) and (62.49), and we obtain now for E^2 the values

$$E^2 = 0, \quad E_N^2 = 4 + 4\omega(N + 3) \quad \text{if } s = 0, \quad (62.60a)$$

$$E^2 = 0, \quad E_N^2 = 4 + 4\omega(N + 1) \quad \text{if } s = 1. \quad (62.60b)$$

Disregarding the cockroach nest states $E^2 = 0$, when we combine the spectrum of Eq. (62.59) with that of its super partner in Eq. (62.60), we get an expression of the form

$$E_N^2 = 4 + 4\omega(N + \nu), \quad \nu = 0, 1, 2, 3, \quad (62.61)$$

and this is illustrated in Fig. XII.2 where the ordinate is E^2 , and in the abscissa we have both the values $\nu = 0, 1, 2, 3$, as well as those of the corresponding spin $s = 0$ or 1.

The eigenstates of our problem, together with its supersymmetric partner, continue to be given by the ket (62.16) but now we have to add to it the index ν , i.e.,

$$|N(\ell, s)jm\rangle_\nu, \quad (62.62)$$

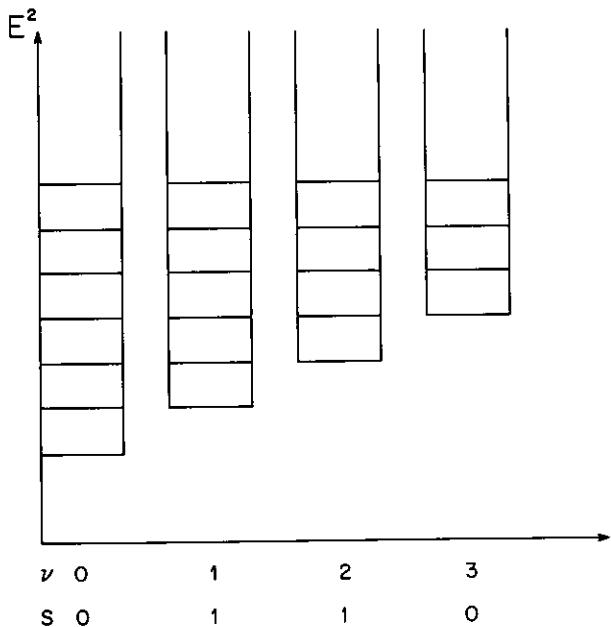


Figure XII.2. Energy levels of the two body relativistic problem with a Dirac oscillator interaction as given in formula (62.61) involving states of both frequencies ω and $-\omega$.

where $\nu = 0, 2$ indicates that the eigenstates correspond to our original equation while $\nu = 1, 3$ imply that it is now associated with the super partner equation in which ω has been replaced by $-\omega$. The relations between ν and the spin $s = 0, 1$ is shown in Fig. XII.2.

We shall now discuss a caricature of the state (62.62) in terms of boson and fermion creation and annihilation operators, where the former will be the $\eta_q, \xi^{q'}, q, q' = 1, 0, -1$ of (62.6) while the latter will be denoted by $a_\sigma, b^{\sigma'}, \sigma, \sigma' = 1, 0, -1$ and they satisfy the anticommutation relations

$$\{a_\sigma, a_{\sigma'}\} = 0 \quad (62.63a)$$

$$\{b^\sigma, b^{\sigma'}\} = 0, \quad (62.63b)$$

$$\{a_\sigma, b^{\sigma'}\} = \delta_\sigma^{\sigma'}. \quad (62.63c)$$

All the states in our caricature will be indicated by round kets and for the boson part they will have the form given in (8.16), i.e.,

$$|N\ell\mu\rangle = A_{N\ell}(\eta \cdot \eta)^{(N-\ell)/2} \mathcal{Y}_{\ell\mu}(\eta)|0\rangle, \quad (62.64a)$$

$$A_{N\ell} = (-1)^{(N-\ell)/2} \sqrt{4\pi}$$

$$\times [(N + \ell + 1)!!(N - \ell)!!]^{-1/2}, \quad (62.64b)$$

where $\mathcal{Y}_{\ell M}(\eta)$ is solid spherical harmonic, i.e., $\mathcal{Y}_{\ell M}(r) = r^\ell Y_{\ell M}(\theta, \phi)$ and $|0\rangle$ is the ground state.

For the fermion part we can also consider polynomial in the $a_\sigma, \sigma = 1, 0, -1$ acting on a ground state $|0\rangle$, but as $a_\sigma a_{\sigma'} = -a_{\sigma'} a_\sigma$ we can have only four of them, which we denote by $|\nu s\sigma\rangle$ and which are

$$|000\rangle = |0\rangle, \quad (62.65a)$$

$$|11\sigma\rangle = a_\sigma|0\rangle, \quad \sigma = 1, 0, -1, \quad (62.65b)$$

$$|21\sigma\rangle = \sum_{\sigma', \sigma''=-1}^1 (-1)^\sigma \epsilon^{-\sigma\sigma'\sigma''} a_{\sigma'} a_{\sigma''}|0\rangle, \quad \sigma = 1, 0, -1 \quad (62.65c)$$

$$|300\rangle = a_1 a_0 a_{-1}|0\rangle, \quad (62.65d)$$

where $\epsilon^{-\sigma\sigma'\sigma''}$ is the totally antisymmetric symbol.

The states of our caricature that correspond to those of (62.62) are then

$$|N\nu(\ell, s)jm\rangle = \sum_{\mu, \sigma} [\sqrt{2j+1}(-1)^{\ell-s+m} \times \binom{\ell}{\mu} \binom{s}{\sigma} \binom{j}{-m} |N\ell\mu\rangle |\nu s\sigma\rangle]. \quad (62.66)$$

It is now a simple matter to derive a Hamiltonian for which the kets (62.66) are eigenkets. As in (62.6), we denote with bold face letters η, ξ the vectors whose components are $\eta_q, \xi^{q'} = (-1)^{q'} \xi_{-q'}$, and we shall use bold face letters a, b for vectors whose components are $a_\sigma, b^{\sigma'} = (-1)^{\sigma'} b_{-\sigma'}$.

The Hamiltonian of which the ket (62.66) is an eigenstate will then have the form

$$\hat{\mathcal{H}} \equiv \eta \cdot \xi + a \cdot b, \quad (62.67)$$

and its corresponding eigenvalue will be

$$\mathcal{H} = N + \nu. \quad (62.68)$$

It is now simple to see that symmetry superalgebra of the Hamiltonian (62.67) is given by the even generators

$$C_q^{q'} = \eta_q \xi^{q'}, \quad (62.69a)$$

$$C_\sigma^{\sigma'} = a_\sigma b^{\sigma'}, \quad (62.69b)$$

and the odd ones

$$T_q^\sigma = \eta_q b^\sigma, \quad (62.70a)$$

$$U_\sigma^q = a_\sigma \xi^q, \quad (62.70b)$$

whose commutation and anticommutation rules, designated by square and curly brackets, respectively, are the following:

$$[C_q^{q'}, C_{q''}^{q''}] = C_q^{q'''} \delta_{q''}^{q'} - C_{q''}^{q'''} \delta_q^{q''}, \quad (62.71a)$$

$$[C_\sigma^{\sigma'}, C_{\sigma''}^{\sigma''}] = C_\sigma^{\sigma'''} \delta_{\sigma''}^{\sigma'} - C_{\sigma''}^{\sigma'''} \delta_\sigma^{\sigma''}, \quad (62.71b)$$

$$[C_q^{q'}, T_{q''}^\sigma] = T_q^\sigma \delta_{q''}^{q'}, \quad (62.71c)$$

$$[C_q^{q'}, U_\sigma^{q''}] = -U_\sigma^{q'} \delta_q^{q''}, \quad (62.71d)$$

$$[C_\sigma^{\sigma'}, T_q^{\sigma''}] = -T_q^{\sigma'} \delta_\sigma^{\sigma''}, \quad (62.71e)$$

$$[C_\sigma^{\sigma'}, U_\sigma^{q''}] = U_\sigma^q \delta_{\sigma''}^{q'}, \quad (62.71f)$$

$$\left\{ T_q^\sigma, T_{q'}^{\sigma'} \right\} = 0, \quad (62.71g)$$

$$\left\{ U_\sigma^q, U_{\sigma'}^{q'} \right\} = 0, \quad (62.71h)$$

$$\left\{ T_q^\sigma, U_{\sigma'}^{q'} \right\} = C_q^{q'} \delta_\sigma^{\sigma'} + C_{\sigma'}^{\sigma'} \delta_q^{q'}. \quad (62.71i)$$

As all of these generators obviously commute with the operator \hat{H} of (62.67), we clearly have here a superalgebra $u(3/3)$ which fully explains the accidental degeneracy present in the levels of Fig. XII.2. The Lie algebras $u(3)$ whose generators are $C_q^{q'}$, $C_\sigma^{\sigma'}$ will connect all states of definite energy in a given column of Fig. XII.2, while the odd generators T_q^σ and U_σ^q , are the ones that, within a given energy level, takes us from one column to next in Fig. XII.2.

It is now of interest to see what is the form of the fermion operators a , b when acting directly on the states (62.62) rather than on its caricature (62.66). It has been shown [12] that these are the matrix operators

$$\tilde{a} = \begin{bmatrix} 0 & 0 & 0 & S \\ S' & 0 & 0 & 0 \\ 0 & S & 0 & 0 \\ 0 & 0 & S' & 0 \end{bmatrix}, \quad (62.72a)$$

$$\tilde{b} = \begin{bmatrix} 0 & S' & 0 & 0 \\ 0 & 0 & S & 0 \\ 0 & 0 & 0 & S' \\ S & 0 & 0 & 0 \end{bmatrix}, \quad (62.72b)$$

where

$$S = \frac{1}{2}(\sigma_1 + \sigma_2), \quad (62.73a)$$

$$S' = \frac{1}{2}(\sigma_1 - \sigma_2), \quad (62.73b)$$

and they act on the spin states $\chi_{s\sigma}$ of (62.15) in the two-body system with a Dirac oscillator interaction, as well as in its super symmetric partner, in the way a , b act on the kets $|\nu s\sigma\rangle$ of (62.65). Furthermore they satisfy the standard anticommutation relations (62.63) for fermion operators.

This means that the generators of the supersymmetry algebra of our problem could be obtained from (62.69,70), just by keeping the same meaning for η , ξ but replacing a , b by \tilde{a} , \tilde{b} of (62.72).

Thus we have completed our discussion of the symmetry algebras and superalgebras for Eq. (62.4) with both values (62.3a,b) of the term B .

As a last point we would like to stress the differences between the equations (62.4) when $B = \beta_1 \beta_2$ and $B = \beta_1 \beta_2 \gamma_{51} \gamma_{52}$ by taking their non-relativistic limit. This implies considering Eqs. (62.9) and (62.38,39) as systems of two equations in (ϕ_+, ϕ_-) and so we could eliminate the ϕ_- between them to get a single equation for ϕ_+ , that contains terms in ω and ω^2 . The nonrelativistic limit is achieved, in our units, when $\omega \ll 1$ and thus the term in ω^2 can be disregarded. In the resulting equation we note that $E^2 - 4 = (E+2)(E-2) \simeq 4\epsilon$, as E is very close to the rest mass of the two particles given by 2, and the nonrelativistic energy is $\epsilon = E - 2$. Thus we obtain for the nonrelativistic Hamiltonian \hat{H} when $B = \beta_1 \beta_2$ the expression

$$H = \omega(\eta \cdot \xi - L \cdot S), \quad (62.74a)$$

while for $B = \beta_1 \beta_2 \gamma_{51} \gamma_{52}$, if we denote it by H' , we have

$$H' = \omega(\eta \cdot \xi + S^2). \quad (62.74b)$$

Clearly H gives a correlation between the orbital and spin angular momenta, while H' does not, and though both Hamiltonians contain the oscillator term $\omega(\eta \cdot \xi)$, they differ in what is added to it.

63 Mass Spectra of the Particle-Antiparticle System with a Dirac Oscillator Interaction

While in the previous section we discussed the two-body system with a Dirac oscillator interaction, and solved it for the eigenvalues and eigenstates in an explicit analytic fashion, we did not give any specific application.

The most obvious one would be mesons formed by a quark and its antiquark, as the two particles would have the same mass. There is though the question of what is the equation for an antiparticle, if we know that the

particle moves in a Dirac oscillator potential. We shall proceed to show that if to the particle corresponds the frequency ω , the antiparticle will obey the same type of equation but with ω replaced by $-\omega$. Thus the relations between particle and antiparticle in a Dirac oscillator potential, is of the same type as that between electron and positron, where the charge has to be changed from e to $-e$.

After the above discussion we shall proceed to derive the equation of the particle-antiparticle system with a Dirac oscillator interaction. Unfortunately this equation has not an exact solution, but we can use perturbative methods to obtain information about its behavior.

We shall discuss all the information that the method in the previous paragraph provides and apply part of it for a qualitative approach to the mass formula of some mesons.

a) The Dirac oscillator equation for an antiparticle

The solution of the Dirac oscillator equation (59.3) was considered in section 59 when we were dealing with positive energies, so a more correct expression for (59.4) would be

$$\psi^+ = \begin{bmatrix} \psi_1^+ \\ \psi_2^+ \end{bmatrix} \exp(-iEx^0), \quad (63.1)$$

as we implicitly assumed that E was positive, so we added + signs to the solution. All the explicit expressions of ψ_1 in (59.9) and ψ_2 in (59.17) apply then to this positive energy solution and, in particular, we shall refer to the ket (59.9) by the shorthand notation ϕ , i.e.,

$$\phi \equiv |N(\ell, \frac{1}{2})jm\rangle. \quad (63.2)$$

Thus the wave function for a particle ψ_p is this positive energy solution of (59.3), so we have from (59.4,9,15) and (63.2) that it is given by

$$\psi_p \equiv \psi^+ = \begin{bmatrix} \phi \\ (E+1)^{-1}[\sigma \cdot (\mathbf{p} - i\omega \mathbf{r})]\phi \end{bmatrix}. \quad (63.3)$$

Now we turn our attention to negative energy states where

$$\psi^- = \begin{bmatrix} \psi_1^- \\ \psi_2^- \end{bmatrix} \exp(iEx^0), \quad (63.4)$$

so that applying to it Eq.(59.3) we get

$$-(E+1)\psi_1^- = [\sigma \cdot (\mathbf{p} + i\omega \mathbf{r})]\psi_2^-, \quad (63.5a)$$

$$(-E+1)\psi_2^- = [\sigma \cdot (\mathbf{p} - i\omega \mathbf{r})]\psi_1^-, \quad (63.5b)$$

and eliminating ψ_1^- between these two equations we get that ψ_2^- is a solution of the equation

$$(E^2 - 1)\psi_2^- = (p^2 + \omega^2 r^2 + 3\omega + 4\omega \mathbf{L} \cdot \mathbf{S})\psi_2^-, \quad (63.6)$$

so while the equation is different from the one of ψ_1^+ in (59.9) the solution is still given by the ϕ of (63.2).

For the antiparticle solution ψ_a we follow Bjorken and Drell [13] by taking the conjugate of ψ^- of (63.4) and apply to it the matrix

$$i\gamma_2 = i\beta\alpha_2 = i \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix}, \quad (63.7)$$

thus getting

$$\psi_a \equiv i\gamma_2\psi^{-*} = \left[(E+1)^{-1}\sigma \cdot (\mathbf{p} + i\omega \mathbf{r})(i\sigma_2\phi^*) \right] \exp(-iEx^0), \quad (63.8)$$

as

$$(-i\sigma_2)\sigma^*(-i\sigma_2) = \sigma, \quad (63.9a)$$

$$(-i\sigma_2)(i\sigma_2) = I. \quad (63.9b)$$

Furthermore as the χ_σ in (59.9) is the function corresponding to spin 1/2 and projection σ , we have that

$$i\sigma_2\chi_{1/2} = -\chi_{-1/2}, \quad (63.10a)$$

$$i\sigma_2\chi_{-1/2} = \chi_{1/2}, \quad (63.10b)$$

so finally

$$\begin{aligned} i\sigma_2\phi^* &= R_{N\ell}(\sqrt{\omega}r) \sum_{\sigma=-1/2}^{1/2} \sqrt{2j+1}(-1)^\ell \\ &\times \begin{pmatrix} \ell & \frac{1}{2} & j \\ m-\sigma & \sigma & -m \end{pmatrix} Y_{\ell,-m+\sigma}(\theta, \varphi)\chi_{-\sigma}, \end{aligned} \quad (63.11)$$

so that changing σ, m into $-\sigma, -m$, and using properties of the $3j$ coefficients [8], we obtain

$$i\sigma_2\phi^* = (-1)^{m+j-\ell}\phi. \quad (63.12)$$

Thus (except for the phase factor $(-1)^{m+j-\ell}$ which is irrelevant), we see from (63.6,8) that the state ψ_a of the antiparticle is a solution of the Dirac oscillator Eq. (59.3) if we replace ω by $-\omega$.

b) Equation for the particle-antiparticle system with a Dirac oscillator interaction and its perturbative solution

In Eq. (62.52) we wrote the Poincaré invariant equation for a system of two particles with a Dirac oscillator interaction of frequency ω . The Poincaré invariance of the problem would not be affected if instead of each coordinate $x'_{\perp \mu_1}, x'_{\perp \mu_2}$ being associated with the same frequency ω they would have their own frequency ω_1, ω_2 , i.e., if Eq. (62.52) becomes

$$\left\{ \sum_{s=1}^2 \Gamma_s [\gamma_s^\mu (p_{\mu s} - i\omega_s x'_{\perp \mu s} \Gamma) + 1] \right\} \psi = 0. \quad (63.13)$$

From the discussion of the previous subsection this will become the Poincaré invariant equation of a particle-antiparticle system with a Dirac oscillator interaction of frequency ω if we have the relation

$$\omega_1 = -\omega_2 \equiv \omega. \quad (63.14)$$

If we now pass to the frame of reference where the center of mass is at rest, by a procedure entirely analogous to the one followed between Eqs. (62.52) and (62.55), we arrive at the equation

$$\{(\alpha_1 - \alpha_2) \cdot p - i(\omega/2)[(\alpha_1 + \alpha_2) \cdot r]\beta_1\beta_2 + \beta_1 + \beta_2\} \psi = E\psi, \quad (63.15)$$

where, as before, $p = (1/2)(p_1 - p_2)$, $r = (x_1 - x_2)$.

Expressing this equation explicitly as in (62.5) and using the creation and annihilation operators of (62.6), Eq. (63.15), with ψ in its four vector form (61.13), becomes

$$i\sqrt{\omega} \begin{bmatrix} \sigma_1 \cdot \eta & \sigma_2 \cdot \xi \\ \sigma_2 \cdot \xi & \sigma_1 \cdot \eta \end{bmatrix} \begin{bmatrix} \psi_{21} \\ \psi_{12} \end{bmatrix} = \begin{bmatrix} (E-2)\psi_{11} \\ (E+2)\psi_{22} \end{bmatrix}, \quad (63.16a)$$

$$-i\sqrt{\omega} \begin{bmatrix} \sigma_1 \cdot \xi & \sigma_2 \cdot \eta \\ \sigma_2 \cdot \eta & \sigma_1 \cdot \xi \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{22} \end{bmatrix} = E \begin{bmatrix} \psi_{21} \\ \psi_{12} \end{bmatrix}. \quad (63.16b)$$

Multiplying (58.16a) by E and introducing in it (58.16b) we get a single equation involving only ψ_{11}, ψ_{22} . Passing then to the functions (ϕ_+, ϕ_-) through the transformation (61.15) we get finally the equation

$$\omega \begin{bmatrix} A - D & 0 \\ 0 & A + D \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = \begin{bmatrix} E^2 & -2E \\ -2E & E^2 \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix}, \quad (63.17)$$

where

$$A \equiv 2\eta \cdot \xi + 3 - \mathbf{L} \cdot (\sigma_1 - \sigma_2), \quad (63.18a)$$

$$D \equiv 2(\mathbf{S} \cdot \eta)^2 + 2(\mathbf{S} \cdot \xi)^2 - (\eta \cdot \eta) - (\xi \cdot \xi), \quad (63.18b)$$

where η, ξ are given by (62.6) and \mathbf{L}, \mathbf{S} by (62.10).

Writing the two equations for ϕ_+, ϕ_- implied by (63.17), we can eliminate ϕ_- between them and obtain for ϕ_+ , which we will now designate simply as ϕ , that it satisfies the equation

$$[E^4 - (4 + 2\omega A)E^2 + \omega^2(A^2 - D^2 - AD + DA)]\phi = 0. \quad (63.19)$$

Unfortunately, because of the term D of (63.18b), this problem is not exactly soluble as was the case of two particles, i.e., when $\omega_1 = \omega_2 = \omega$, discussed in the previous section. We note though that the operator in (63.19) contains the frequency ω as a parameter. As this frequency is given in units of the rest mass 1 of the particle, we expect ω to be small as compared with 1, as is the case in nuclear physics. We can then begin by disregarding the term in ω^2 and so our equation becomes

$$E^2 [E^2 - (4 + 2A\omega)]\phi = 0, \quad (63.20)$$

so our first objective will be to find the eigenstates and eigenvalues of the operator A given by (63.18a).

To achieve our purpose we start by introducing the ket $|N(\ell, s)jm\rangle$ of (62.16). We note from (63.18) that the operators in (63.19) are invariant under reflections, i.e., change of η, ξ into $-\eta, -\xi$ and thus the parity of the states (62.16), which is $(-1)^\ell$, is a good quantum number. Considering then separately the states (62.16) in which $\ell = j$, and those in which $\ell = j \pm 1$, we find by straightforward Racah algebra [8] that the eigenstates of A of (63.18a), which we shall denote by ϕ_0 , are

$$\phi_0 \equiv (1/\sqrt{2}) \left[|N(j, 0)jm\rangle \pm |N(j, 1)jm\rangle \right] \quad \text{for parity } (-1)^j, \quad (63.21a)$$

$$\phi_0 \equiv |N(j \pm 1, 1)jm\rangle \quad \text{for parity } -(-1)^j. \quad (63.21b)$$

The corresponding eigenvalues of E^2 , which we denote by E_0^2 , are given by

$$E_0^2 = 4 + 2\omega \left\{ (2N + 3) \pm [j(j + 1)]^{1/2} \right\} \quad (63.22a)$$

for parity $(-1)^j$, while for parity $-(-1)^j$ we get

$$E_0^2 = 4 + 2\omega(2N + 3), \quad (63.22b)$$

and thus we have a complete solution of the problem (63.20).

Our interest though is in Eq. (63.19) which we can solve by a perturbation procedure. We first define

$$W \equiv E^2, \quad (63.23a)$$

$$H_0 = 4 + 2A\omega, \quad (63.23b)$$

$$H' = \omega^2(A^2 - D^2 - AD + DA), \quad (63.23c)$$

so equation (63.19) becomes

$$(W^2 - WH_0 + H')\phi = 0. \quad (63.24)$$

We then, as for example in Schiff book [14], replace H' by $\lambda H'$ where λ is a parameter and write

$$W = W_0 + \lambda W_1 + \lambda^2 W_2 + \dots, \quad (63.25a)$$

$$\phi = \phi_0 + \lambda \phi_1 + \lambda^2 \phi_2 + \dots, \quad (63.25b)$$

where $W_0 = E_0^2$ of (63.22) and ϕ_0 is given by (63.21).

From (63.25) we obtain

$$W^2 = W_0^2 + \lambda(2W_0W_1) + \lambda^2(2W_0W_2 + W_1^2) + \dots, \quad (63.25c)$$

so that using (63.25) we see that, up to first order in λ , (63.24) takes the form

$$\begin{aligned} & \left[W_0(W_0 - H_0)\phi_0 \right] + \lambda \left[(2W_0W_1 - W_1H_0 + H')\phi_0 \right. \\ & \left. + W_0(W_0 - H_0)\phi_1 \right] + \dots = 0, \end{aligned} \quad (63.26)$$

where each of the square brackets must vanish [14]. For the first one this is automatic as from (63.20) we have

$$H_0\phi_0 = W_0\phi_0. \quad (63.27)$$

From the second square bracket, when we take its scalar product [14] with ϕ_0 , we obtain

$$W_1 = -W_0^{-1}(\phi_0, H'\phi_0), \quad (63.28)$$

where we made use of the hermitian character of H_0 and of Eq. (63.27).

Thus to first order in perturbation theory, when we take, as usual [14], $\lambda = 1$, we have that

$$E^2 = E_0^2 - E_0^{-2}(\phi_0, H'\phi_0) + \dots, \quad (63.29)$$

where E_0^2 is given by (63.22), ϕ_0 by (63.21) and H' is (63.23c). In the next subsection we calculate this E^2 explicitly.

c) Square of the mass spectra of the particle-antiparticle system

To determine the square of the mass E^2 , given to first order perturbation theory by (63.29), we need to calculate the scalar product $(\phi_0, H'\phi_0)$. As ϕ_0 has a definite number of quanta N , which is indicated in (63.21), we need only to consider that part of H' in (63.23c) that does not change the number of quanta. The terms AD, DA in (63.23) change the number of quanta by ± 2 , as indicated in (63.18), so we can disregard them. The A^2 is diagonal in the basis ϕ_0 of (63.21) and its contribution to the scalar product in (63.28) is

$$(\phi_0, A^2\phi_0) = \left\{ (2N+3) \pm [j(j+1)]^{1/2} \right\}^2 \quad \text{for parity } (-1)^j, \quad (63.30a)$$

$$(\phi_0, A^2\phi_0) = (2N+3)^2 \quad \text{for parity } (-1)^j. \quad (63.30b)$$

For the D^2 operator, where D is given by (63.18b), the only terms that contribute to its expectation value with respect to ϕ_0 , i.e., that do not change the number of quanta N , are

$$\begin{aligned} & 4(S \cdot \eta)^2(S \cdot \xi)^2 + 4(S \cdot \xi)^2(S \cdot \eta)^2 - 2(S \cdot \eta)^2(\xi \cdot \xi) \\ & - 2(S \cdot \xi)^2(\eta \cdot \eta) - 2(\eta \cdot \eta)(S \cdot \xi)^2 - 2(\xi \cdot \xi)(S \cdot \eta)^2 \\ & + (\eta \cdot \eta)(\xi \cdot \xi) + (\xi \cdot \xi)(\eta \cdot \eta). \end{aligned} \quad (63.31)$$

To evaluate the matrix element $(\phi_0, H'\phi_0)$ we need then to determine the matrix elements of $(S \cdot \eta)^2, (S \cdot \xi)^2, (\eta \cdot \eta), (\xi \cdot \xi)$ with respect to states of the form $|N(\ell, s)jm\rangle$ of (62.16). This is done using results for the matrix elements of $(S \cdot \eta), (S \cdot \xi)$ given in (62.25,32) as well as the operator form of the harmonic oscillator states in (62.64).

We finally arrive at the following results for the E^2 of (63.29): For the states of parity $(-1)^j$, E^2 can be expressed as a function of N, j, ω , using both signs \pm in the ϕ_0 of (63.21a), i.e.,

$$\begin{aligned} E_{\pm}^2(N, j, \omega) = & 4 + 2\omega \left\{ (2N+3) \pm [j(j+1)]^{1/2} \right\} \\ & - (\omega^2/4) \left\{ [(2N+3) \pm j^{1/2}(j+1)^{1/2}]^2 \right. \\ & \left. - 2[N(N+3) - j(j+1) + 3] \right\} + \dots \end{aligned} \quad (63.32)$$

For the states of parity $-(-1)^j$, the two cases of orbital angular momentum $\ell = j+1$ or $\ell = j-1$, have to be written separately. We shall distinguish

them from (63.32) by putting a bar above the E^2 and an index + or - when ℓ is respectively $j+1$ or $j-1$. Thus we obtain

$$\bar{E}_+^2 = 4 + 2\omega(2N+3) - (\omega^2/4) \\ \times \{(2N+3)^2 - 2[j(j-1) + N(N+3)+1]\} + \dots, \quad (63.33a)$$

$$\bar{E}_-^2 = 4 + 2\omega(2N+3) - (\omega^2/4) \\ \times \{(2N+3)^2 - 2[j(j+3) + N(N+3)+3]\} + \dots \quad (63.33b)$$

In all of these cases we keep only terms up to ω^2 so that E_0^{-2} appearing as a coefficient of the scalar product in (63.29) is replaced by (1/4). Note furthermore that as $N = 2n + \ell$ where ℓ is the *orbital* angular momentum, we see that for $E_{\pm}^2(N, j, \omega)$ of (63.32) the N takes the values $N = j, j+2, j+4, \dots$. On the other hand for $\bar{E}_{\pm}^2(N, j, \omega)$ of (63.33a) N takes the values $N = j+1, j+3, j+5, \dots$, while for $\bar{E}_{\pm}^2(N, j, \omega)$ of (63.33b) we have $N = j-1, j+1, j+3, j+5, \dots$

In Fig. XII.3 we graph E_{\pm}^2 of (63.32) for $\omega = 0.1$ as function of j , indicating the sign \pm to which the level corresponds on its left hand side while on the right hand side we give the value of N . Note that when $j = 0$ the state $|N(0, 1)00\rangle$ does not exist so that the normalized ϕ_0 of (63.21a) reduces to $|N(0, 0)00\rangle$. In this case the spin is 0 as indicated in the left hand side of the level $j = 0$, and not the mixture \pm in (63.21a).

In Fig. XII.4 we graph \bar{E}_{\pm}^2 of (63.33) for $\omega = 0.1$ as function of j . The orbital angular momentum $\ell = j \pm 1$ is indicated on the left of the levels and the total number of quanta N is given on the right. Note that for $j = 0$, $|N(-1, 1)00\rangle$ does not exist so that we have only $|N(1, 1)00\rangle$ corresponding to $\ell = 1$ indicated on the left hand side of the levels with $j = 0$. Also the levels with $N = \ell = j-1$ are unique as indicated in the corresponding left hand side of the levels. For the other states $|N(j \pm 1, 1)jm\rangle$ both values $\ell = j+1$ and $j-1$ are possible, and because of the first order corrections, i.e., the term in ω^2 of (63.33) they are separated by $\omega^2(2j+1)$. In Fig. XII.4 we give on the left hand side the values $\ell = j+1$ and $\ell = j-1$ of the paired levels.

The parity denoted by a script \mathcal{P} is given in all figures, i.e., $\mathcal{P} = (-1)^j$ or $\mathcal{P} = -(-1)^j$.

In the next subsection we discuss the comparison of our results with squares of the mass spectra for non-strange mesons [15].

d) Comparison with the meson spectra

On page 37 of reference [15] there is a Meson Summary Table in which, in the first two columns, are given the non-strange mesons with the code name (a single letter with an index indicating the total angular momentum j),

mass E in MeV, j , isospin I , and parity defined there [15] as $P = -(-1)^{\ell}$, as well as a charge conjugation number $C = (-1)^{\ell+s}$, where ℓ is the orbital angular momentum and s the total spin of the quark-antiquark system.

From the above information we can get the square of the mass E^2 in units GeV^2 , the j, s, I as well as $(-1)^{\ell}$, so that, $\ell = j$ or $\ell = j \pm 1$. As mentioned before our notation for parity will be the script $\mathcal{P} = (-1)^{\ell}$, i.e., $\mathcal{P} = (-1)^j$ or $-(-1)^j$.

The information given in the previous paragraph is summarized in Figs. XII.5-XII.8, where in the abscissa we have $j = 0, 1, 2, 3, 4, 5$ and E^2 in the ordinate. We note first that for comparison with the particle-antiparticle system, with a Dirac oscillator interaction, we have divided the information according to parity $\mathcal{P} = (-1)^j$ or $-(-1)^j$ in Figs. XII.5-XII.6 or Figs. XII.7-XII.8 as \mathcal{P} is an integral of motion of our problem. Furthermore the isospin $I = 0, 1$ is completely independent from the Poincaré group and thus of the analysis in the previous sections. We could then consider that in our theoretical E_{\pm}^2 of (63.32) or \bar{E}_{\pm}^2 of (63.33), ω is a function of I and another parameter could be added to those in $E_{\pm}^2, \bar{E}_{\pm}^2$. Thus it is convenient to graph separately the levels for $I = 1, \mathcal{P} = (-1)^j$ (Fig. XII.5); $I = 0, \mathcal{P} = (-1)^j$ (Fig. XII.6); $I = 1, \mathcal{P} = -(-1)^j$ (Fig. XII.7); and $I = 0, \mathcal{P} = -(-1)^j$ (Fig. XII.8).

In Figs. XII.5-XII.8 we put on the left hand side the name of the meson and where there are several of the same name we distinguish them by primes, i.e., π_j, π'_j, π''_j etc. In Figs. XII.5 and XII.6 we put on the right hand side the total spin $s = 0$ or 1 and furthermore we differentiate the two values by using either a full or dashed line. In Figs. XII.7 and XII.8 only the names of the mesons appear on the levels as the spin s is always 1.

We now wish to make a qualitative comparison between the theoretical Figs. XII.3 and XII.4 and the experimental ones for mesons in Figs. XII.5-XII.8.

We begin with parity $\mathcal{P} = (-1)^j$ where we should compare Fig. XII.3 with Figs. XII.5 and XII.6. For angular momentum $j = 0$ the comparison in Figs. XII.1 and XII.3 is quite good and the spin is $s = 0$. For all other levels we cannot compare because in Fig. XII.5 they have definite spin, while in Fig. XII.3 we have 50% each of admixtures of $s = 0$ and $s = 1$, in or out of phase, as shown in (63.21a). This clearly shows the need to add other interactions in our equation (63.13) that are Poincaré invariant, which were discussed in reference [16]. Note also that even for $j = 0$ the comparison between Figs. XII.3 and XII.6 is not good, even if we change the scale in Fig. XII.3, but this can be attributed to the fact that the η_0 mesons may have an admixture of $s\bar{s}$ where s has different mass from u, d .

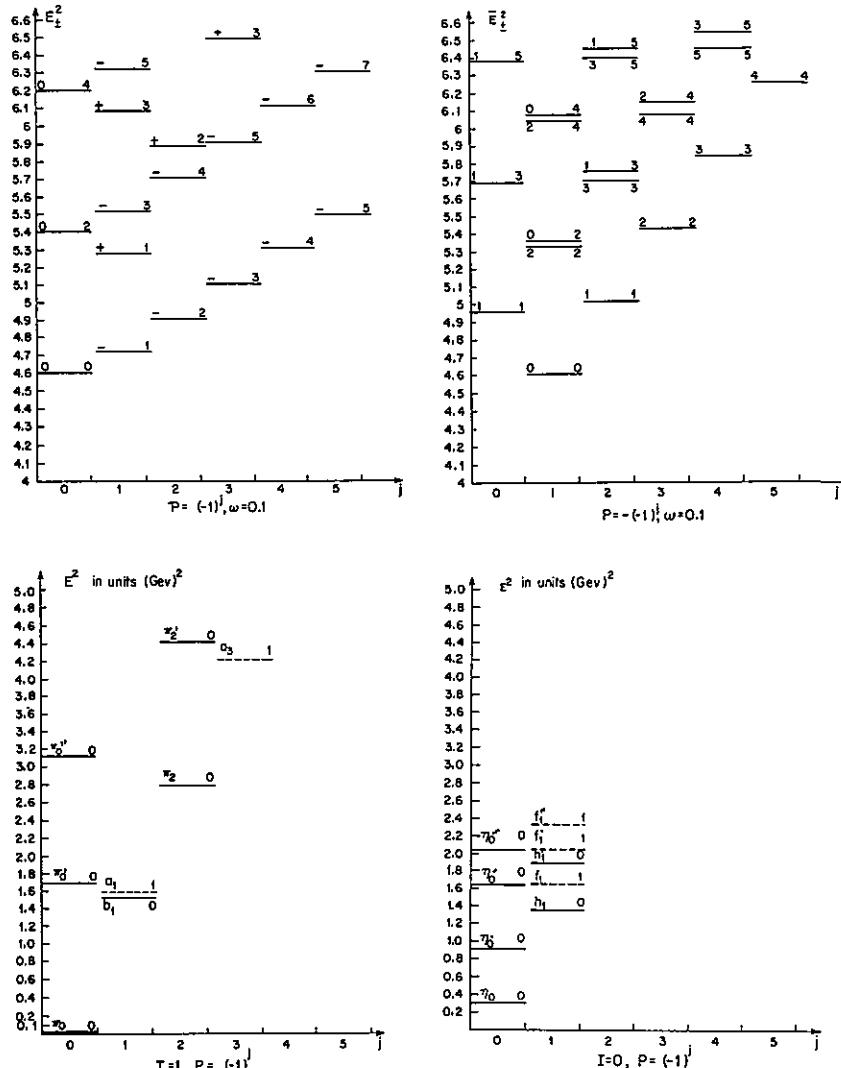


Figure XII.3 (top left). In the abscissa we give the value of j and in the ordinate that of E_{\pm}^2 determined by (63.32). The value of N is indicated on the right and \pm on the left except when $j = 0$, when the spin, given on the left, is also 0. Figure XII.4 (top right). In the abscissa we give the value of j and in the ordinate that of \bar{E}_{\pm}^2 determined by (63.33). The value of N is given on the right and those of $l = j \pm 1$ on the left. Figure XII.5 (bottom left). The square of the masses of the non-strange mesons are given as functions of j for isospin $I = 1$ and parity $P = (-1)^j$. The name of the meson is given on the left with an index j and upper primes if there are several. Full lines correspond to spin $s = 0$ and dashed to spin 1, as indicated on the right. Figure XII.6 (bottom right). The square of the masses of the non-strange mesons are given as a function of j for isospin $I = 0$ and parity $P = (-1)^j$. The names of the mesons

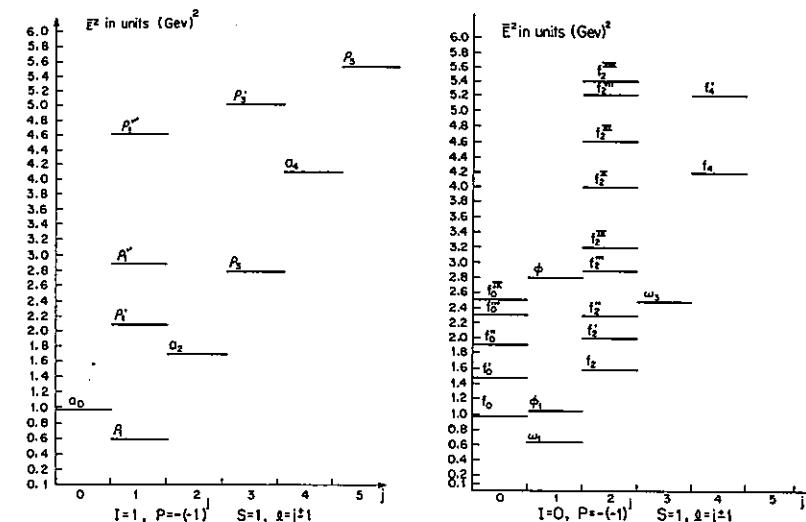


Figure XII.7 (left). The square of the masses of the non-strange mesons are given as a function of j for isospin $I = 1$ and parity $P = -(-1)^j$. The name of the meson is given on the left with an index j and upper primes if there are several. The spin is always 1. Figure XII.8 (right). The square of the masses of the non-strange mesons are given as a function of j for isospin $I = 0$ and parity $P = -(-1)^j$. The name of the meson is given on the left with an index j and upper primes if there are several. The spin is always 1.

Turning now our attention to parity $P = -(-1)^j$ we could compare Fig. XII.4 with Fig. XII.7 or XII.8. In Fig. XII.7, i.e., $I = 1$ the information is sparse though for $j = 1$ we see what may be a pair p'_1, p''_1 which, with a change of scale, could resemble the pair for $j = 1, N = 2$ in Fig. XII.4. This is more noticeable when we compare, for $j = 2$, Fig. XII.4 with Fig. XII.8, where we see a number of pairs, i.e., $N = 3$ corresponding $f'_2, f''_2; N = 5$ to f'''_2, f^{IV}_2 ; and if we had graphed it, $N = 7$ to $f^V_2, f^{VI}_2; N = 9$ to f^{VII}_2, f^{VIII}_2 . Note also that for parity $P = -(-1)^j$ the lowest level in Figs. XII.7 and XII.8 appears for $j = 1$ and not $j = 0$, and this is also true in the theoretical calculations of Fig. XII.4.

Clearly though in all cases we would have to modify our starting hypothesis and we want to do this in a Poincaré invariant way.

There are a number of ways to achieve this objective as indicated in reference [16], but all of them would imply adding Poincaré invariant terms, with arbitrary coefficients, to Eq. (63.13). Thus we would have more arbitrary coefficients than the single ω that we have used so far, and we could adjust the meson spectra better but it could be meaningless. Therefore we

have restricted our analysis to the particle-antiparticle system with Dirac oscillator interaction given by Eq. (63.13).

64 Radial Equation for the Particle-Antiparticle System and a Qualitative Application to Mesons

In the previous section we obtained, in the frame of reference where the center of mass is at rest, Eq. (63.15) which provides eigenvalues of the total energy E , i.e., in our units the masses of the particle-antiparticle system with a Dirac oscillator interaction. This equation can not be solved exactly, but in the previous section we introduced a perturbative method which, while used only up to first order, seems to provide a discrete spectrum when used up to any order.

We shall show in this section, by deriving from Eq. (63.19) its radial part, that actually the spectrum is continuous with resonances that correspond to the bound states mentioned above.

This situation should not surprise us because if we consider the simple Hamiltonian

$$H = \frac{1}{2}(p^2 + x^2) - \epsilon x^4, \quad (64.1)$$

with ϵ positive and small compared to 1, perturbation theory is applicable using harmonic oscillator wave functions and gives rise to bound states. On the other hand if we look at the form of the potential drawn in Fig. XII.9, it is clear that the spectrum is continuous as the potential goes to $-\infty$ at $x = \pm\infty$, but if $\epsilon \ll 1$ it may have narrow resonant states. Thus we shall proceed with the program outlined in the previous paragraph.

a) The radial wave equation

From (63.18) we see that the wave equation (63.19) depends on the spherical coordinates r, θ, φ associated with \mathbf{r} , as well as on derivatives with respect to them and the components σ_{1i}, σ_{2i} , $i = 1, 2, 3$ of the spin operators.

The solution ϕ of (63.19) will also be an eigenstate of the total angular momentum squared J^2 and its projection J_3 , as the operator in the square bracket of (63.19) commutes with J_i , $i = 1, 2, 3$. Furthermore, this operator is invariant under the reflection

$$\mathbf{r} \rightarrow -\mathbf{r}, \quad \mathbf{p} \rightarrow \mathbf{p}, \quad (64.2)$$

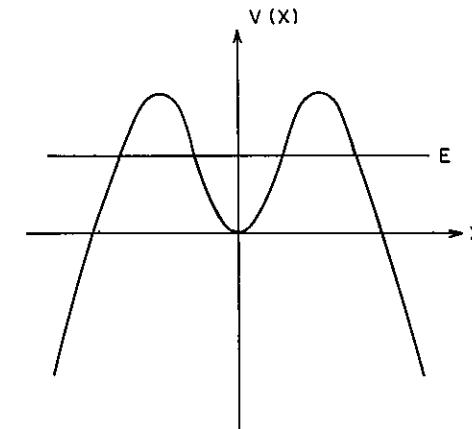


Figure XII.9. Potential $V(x) = (x^2/2) - \epsilon x^4$ with the horizontal line marked E being one of its energy levels. It is clear that the spectrum would be continuous with $-\infty \leq E \leq \infty$, as is also the case for the repulsive oscillator whose wave functions can be obtained analytically. For E close to 0 we can expect narrow resonant states because of the height and width of the barriers when $\epsilon \ll 1$, and the real part of the energy of these states can be obtained by perturbation theory.

so that ϕ will also be characterized by its parity.

We denote now by the ket $|(l, s)jm\rangle$ the angular and spin part of the function ϕ , i.e.,

$$|(l, s)jm\rangle = \sum_{\mu, \sigma} \sqrt{2j+1}(-1)^{\ell-s+m} \begin{pmatrix} \ell & s & j \\ \mu & \sigma & -m \end{pmatrix} Y_{l\mu}(\theta, \varphi) \chi_{s\sigma}, \quad (64.3)$$

where (\cdot) is a $3j$ coefficient, $Y_{l\mu}$ (with $l = j \pm 1$ or j) is a spherical harmonic, and $\chi_{s\sigma}$ is the spin part of the wave function, where $s = 0$ or 1.

From the integrals of motion mentioned above, Eq. (63.19) admits two types of solutions, one of the form

$$\phi = r^{-1} f_0(r) |(j, 0)jm\rangle + r^{-1} f_1(r) |(j, 1)jm\rangle, \quad (64.4)$$

which has parity $(-1)^j$, while the other is

$$\phi = r^{-1} f_+(r) |(j+1, 1)jm\rangle + r^{-1} f_-(r) |(j-1, 1)jm\rangle, \quad (64.5)$$

with parity $-(-1)^j$. The functions $f_0(r), f_1(r)$ or $f_+(r), f_-(r)$, will be determined by radial matrix equations, and we shall proceed to derive the one for $f_s(r)$, $s = 0, 1$.

We note that for our purpose we require the matrix elements

$$\langle(l', s')jm|M|(l, s)jm\rangle, \quad (64.6)$$

where M is either A, D given in (63.18). These matrix elements, besides being functions of r , will also depend on the derivative (d/dr) as the operator $\mathbf{p} = -i\nabla$ appears in A, D . We shall proceed to give all the matrix elements we require for the case when the parity of our state is $(-1)^j$, i.e., when $l = l' = j$ and $s = 0$ or 1

$$\langle(j, s')jm|r^2|(j, s)jm\rangle = \delta_{ss'}r^2, \quad (64.7a)$$

$$\begin{aligned} \langle(j, s')jm|p^2|(j, s)jm\rangle \\ = \delta_{ss'}\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{j(j+1)}{r^2}\right], \end{aligned} \quad (64.7b)$$

$$\begin{aligned} \langle(j, s')jm|\mathbf{L} \cdot (\sigma_1 - \sigma_2)|(j, s)jm\rangle \\ = -(1/2)\left[1 - (-1)^{s+s'}\right]\left[j(j+1)\right]^{1/2}, \end{aligned} \quad (64.7c)$$

$$\begin{aligned} \langle(j, s')jm|(\mathbf{S} \cdot \mathbf{p})^2|(j, s)jm\rangle \\ = \delta_{s'1}\delta_{s1}\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{j(j+1)}{r^2}\right], \end{aligned} \quad (64.7d)$$

$$\langle(j, s')jm|(\mathbf{S} \cdot \mathbf{r})^2|(j, s)jm\rangle = \delta_{s'1}\delta_{s1}r^2. \quad (64.7e)$$

The matrix element (64.7a) is trivial, the one in (64.7b) follows from the expression of the Laplacian in spherical coordinates and the definition (64.3) of the ket $|(l, s)jm\rangle$. The value (64.7c) can be obtained from simple considerations of Racah algebra [8]. The matrix elements (64.7d,e) can be written as

$$\begin{aligned} \langle(j, s')jm|(\mathbf{S} \cdot \mathbf{w})^2|(j, s)jm\rangle &= \sum_{\tau=-1}^1 \langle(j, s')jm|\mathbf{S} \cdot \mathbf{w}|(j+\tau, 1)jm\rangle \\ &\times \langle(j+\tau, 1)jm|\mathbf{S} \cdot \mathbf{w}|(j, s)jm\rangle, \end{aligned} \quad (64.8a)$$

where w is either r or p . The intermediate states on the left hand side of (64.8a) have to be of opposite parity as w is a polar vector, and thus are restricted to $|(j \pm 1, 1)jm\rangle$.

The matrix elements of $(\mathbf{S} \cdot \mathbf{w})$ with $w = r$ and p can be obtained by standard Racah analysis [8] taking into account that the reduced matrix elements of the vector \mathbf{S} with respect to the spin state $|s\sigma\rangle$ is

$$\langle s'|\mathbf{S}|s\rangle = \delta_{s's}[s(s+1)]^{1/2}, \quad (64.8b)$$

while those of the vector \mathbf{r} and \mathbf{p} with respect to orbital angular momentum kets $|\ell m\rangle$ are

$$\langle\ell'|\mathbf{r}|\ell\rangle = r\delta_{\ell',\ell+1}\sqrt{\frac{\ell+1}{2\ell+3}} - r\delta_{\ell',\ell-1}\sqrt{\frac{\ell}{2\ell-1}}, \quad (64.8c)$$

$$\begin{aligned} \langle\ell'|\mathbf{p}|\ell\rangle = \delta_{\ell',\ell+1}\sqrt{\frac{\ell+1}{2\ell+3}}(-i)\left(\frac{d}{dr} - \frac{\ell}{r}\right) \\ - \delta_{\ell',\ell-1}\sqrt{\frac{\ell}{2\ell-1}}(-i)\left(\frac{d}{dr} + \frac{\ell+1}{r}\right), \end{aligned} \quad (64.8d)$$

where the last one was derived also in reference [17]. From (64.8a) we obtain then the results (64.7d,e).

Equation (63.19) becomes then a radial matrix equation of the form

$$\left\{E^4 - (4 + 2A\omega)E^2 + \omega^2(A + D)(A - D)\right\} \begin{bmatrix} f_0(r) \\ f_1(r) \end{bmatrix} = 0, \quad (64.9)$$

where A and D are 2×2 matrices of the form

$$A = \begin{bmatrix} \pi^2 + r^2 & \{j(j+1)\}^{1/2} \\ \{j(j+1)\}^{1/2} & \pi^2 + r^2 \end{bmatrix}, \quad (64.10a)$$

$$D = (\pi^2 - r^2) \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad (64.10b)$$

where

$$\pi^2 \equiv -\frac{d^2}{dr^2} + \frac{j(j+1)}{r^2}, \quad (64.11a)$$

as due to the factor r^{-1} appearing in (64.4) we see that

$$-\left(\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\right)\frac{f_s(r)}{r} = -\frac{1}{r}\frac{d^2f_s(r)}{dr^2}. \quad (64.11b)$$

Written out explicitly, (64.9) gives rise to the two coupled equations

$$\begin{aligned} \left\{(E^2 - 2\omega\pi^2)(E^2 - 2\omega r^2) - 4E^2 + \omega^2[j(j+1)]\right\}f_0(r) \\ = 2\omega[j(j+1)]^{1/2}(E^2 - 2\omega\pi^2)f_1(r), \end{aligned} \quad (64.12a)$$

$$\begin{aligned} \left\{(E^2 - 2\omega r^2)(E^2 - 2\omega\pi^2) - 4E^2 + \omega^2[j(j+1)]\right\}f_1(r) \\ = 2\omega[j(j+1)]^{1/2}(E^2 - 2\omega r^2)f_0(r). \end{aligned} \quad (64.12b)$$

We can use (64.12b) to express $f_0(r)$ in terms of $f_1(r)$, and substituting it in (64.12a) we finally get for $f_1(r)$ the equation

$$\left\{ \mathcal{O} - \left[2E + \omega j^{1/2} (j+1)^{1/2} \right]^2 \right\} \\ \times \left\{ \mathcal{O} - \left[2E - \omega j^{1/2} (j+1)^{1/2} \right]^2 \right\} f_1(r) = 0, \quad (64.13)$$

where

$$\mathcal{O} = (E^2 - 2\omega r^2)(E^2 - 2\omega \pi^2). \quad (64.14)$$

As the operators in the two curly brackets of (64.13) commute, we see that $f_1(r)$ must satisfy the equation

$$\left\{ (E^2 - 2\omega r^2)(E^2 - 2\omega \pi^2) - \left[2E \pm \omega j^{1/2} (j+1)^{1/2} \right]^2 \right\} f(r) = 0, \quad (64.15)$$

where we suppressed the index 1 in $f_1(r)$ and have either a + or - sign in the last square bracket, and π^2 is given by (64.11a). Once $f(r)$, and in the process also E^2 , have been determined, then $f_0(r)$ can be derived from (64.12b) and thus finally ϕ in (64.4) can be obtained explicitly.

A similar analysis can be carried out for the state (64.5) of parity $-(-1)^j$ but the results are more complicated and we will not be presented here.

Equation (64.15) may be rewritten in the following Schrödinger-like form

$$\left\{ -\frac{d^2}{dr^2} + \frac{j(j+1)}{r^2} + \frac{[(E/\omega) \pm \frac{1}{2}\sqrt{j(j+1)}]^2}{(E^2/2\omega) - r^2} \right\} f = \frac{E^2}{2\omega} f, \quad (64.16)$$

which has the interesting property that the effective potential depends on the eigenvalue of the equation. We shall look for solutions of (64.16) which go to zero as $r \rightarrow 0$. Let us suppose $E^2 > 0$. The effective potential entering (64.16) is schematically drawn in Fig. XII.10. The regions $r < E/\sqrt{2\omega}$ and $r > E/\sqrt{2\omega}$ are separated by a Coulomb-like barrier as we have

$$[(E^2/2\omega) - r^2]^{-1} = [(E/\sqrt{2\omega}) + r]^{-1} [(E/\sqrt{2\omega}) - r]^{-1} \\ \simeq [\sqrt{(2/\omega)} E]^{-1} x^{-1} \quad (64.17)$$

when we are close to the barrier and where

$$x \equiv [(E/\sqrt{2\omega}) - r]. \quad (64.18)$$

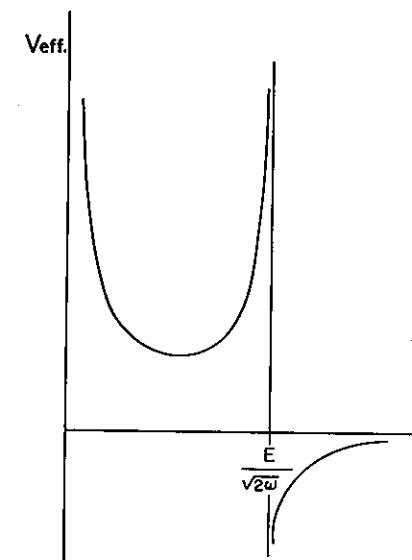


Figure XII.10. Effective potential entering in Eq. (64.16). The Coulomb like barrier at $r = (E/\sqrt{2\omega})$ is penetrable. It means that for positive energies the spectrum is continuous and this potential supports only resonant states (the mesons).

0 is continuous [19]. Nevertheless, as in any barrier problem, there are solutions of (64.16) corresponding to resonant states, *i.e.*, purely outgoing waves. We shall identify these resonant states of quark and antiquark of the same mass, with some types of mesons [19]. The resonant energies are commonly obtained from the asymptotic behavior of the wave function at large distances, *i.e.*,

$$f \simeq A(E) \exp[i(E/\sqrt{2\omega})r] + B(E) \exp[-i(E/\sqrt{2\omega})r], \quad (64.19)$$

and purely outgoing waves imply that

$$B(E) = 0, \quad (64.20)$$

with the complex solutions of this equation determining the resonant energies.

While (64.16) is an ordinary second order differential equation in r , it does not admit an exact solution. In reference [19] we apply what is known as the $1/N$ method [20] to the approximate solution of Eq. (64.16), getting a value close to the real part of the energy one could get from the solution of Eq. (64.20). We refer the reader to reference [19] for the discussion of the $(1/N)$ method as applied to our problem, and here we shall only state some of its results for mesons, and illustrate them with appropriate figures.

of Eq. (64.20). We refer the reader to reference [19] for the discussion of the $(1/N)$ method as applied to our problem, and here we shall only state some of its results for mesons, and illustrate them with appropriate figures.

To begin with we note that our present formalism has only two parameters, the mass m of the quark (which we have taken in this chapter as 1, but whose explicit value in GeV we need to know if we wish to translate our resonant energies to the GeV scale) and the frequency ω of the oscillator.

Thus our predictions can not compare with other models [21], which have a much larger number of parameters. Nevertheless we would like to present the results derived in [19] as compared with scant experimental information and some theoretical results of other authors [21].

We start with the bottom quark b , and its antiquark \bar{b} , i.e., $b\bar{b}$ or bottonium. The mass of this quark is given in reference [21] as $m_b = 4.977$ GeV. The frequency ω is selected to fit the energy gap between the lower and first excited state of bottonium of total angular momentum 0 which, from ref. [21], is expected to be 0.58 GeV and corresponds, when our units are $\hbar = m_b = c = 1$ to the number $\omega_b = 0.062$. Remember that we are only fitting states of parity $(-1)^j$, and in Fig. XII.11 the bold lines are the ones observed experimentally, the dotted lines are the ones calculated in reference [21], the dashed are the results of our calculation [19] with the parameters indicated above and taking the + sign in Eq. (64.16). The abscissa gives the values of the total angular momentum, while the ordinate gives the energies in GeV, starting from the lowest state of the system we are studying, which we put at zero energy.

We pass now to the charm quark c , and its antiquark \bar{c} , i.e., $c\bar{c}$ or charmonium. Again from reference [21] we take the mass $m_c = 1.628$ GeV, while the frequency can be obtained from the energy gap between the two lowest levels for total angular momentum 0, and in units in which $\hbar = m_c = c = 1$ it takes the value $\omega_c = 0.235$. All of the observations of the previous paragraph still apply to Fig. XII.12 corresponding to this problem.

Finally we consider the non-strange quark u and its antiquark \bar{u} . In this case the uncertainty in the value of the mass m_u , is very high, so in reference [19] it is taken as a free parameter together with the frequency ω_u , to fit two experimentally observed magnitudes, the energy gap (1.162 GeV) between the two lowest states of total angular momentum 0, and the pion radius $R_\pi = 0.64$ fm. As in reference [19] also the radius of the mesons can be obtained from the use of $1/N$ approximation method, and from the two data given above we can estimate that

$$m_u = 0.242 \text{ GeV}, \quad (64.21a)$$

$$\omega_u = 7.48. \quad (64.21b)$$

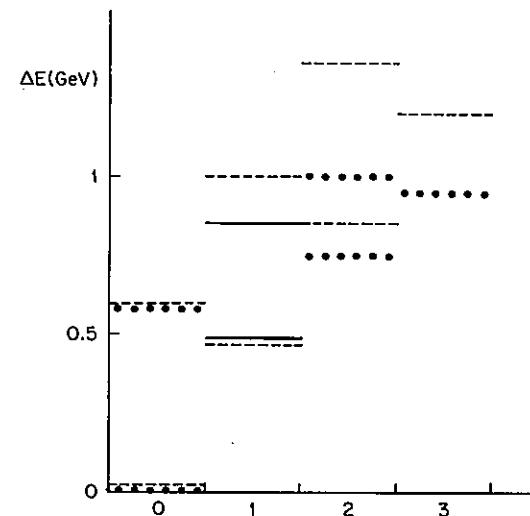


Figure XII.11. Excitation energies ΔE (GeV) of $b\bar{b}$ mesons. The bold lines are experimentally observed levels, dotted lines correspond to calculations of other authors (reference [21]), while our model levels (the E^+ branch) are represented by dashed lines. In the abscissa we indicate the total angular momentum J .

momentum. The full lines give the experimental results from reference [15], the dotted ones are some of those in reference [21], while the dashed ones are the results of our calculations [19]. We note that all the states we consider have parity $(-1)^j$.

We stress again that our model has essentially only the parameter ω , and thus comparison with experiment has to be selective. Thus the radial equation for the quark-antiquark system with a Dirac oscillator interaction can provide only a qualitative approach to the understanding of meson spectra. We note that in reference [19] besides the excitation energies, many other aspects of the quark-antiquark system are discussed.

65 A Relativistic Two-Body Problem with an Interaction Modulated by a Constant Tensor

We considered in section 60 a single relativistic particle in an electromagnetic field and arrived at the Poincaré invariant equation (60.1). In a collaboration with A. del Sol Mesa, we extend it to two particles through an equation of a form similar to (62.52), but now with the coordinates

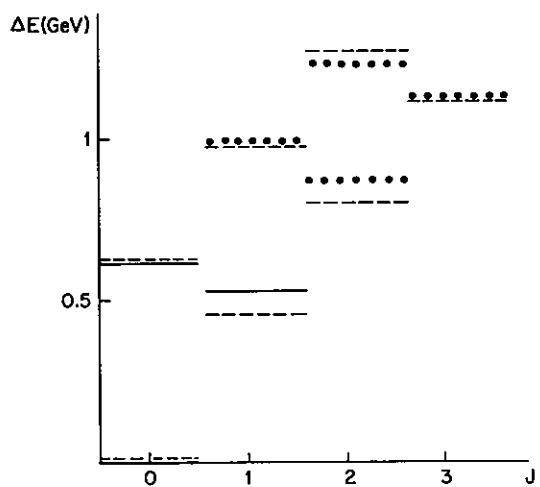


Figure XII.12. Excitation energies ΔE (GeV) of $c\bar{c}$ mesons. The bold lines are experimentally observed levels, dotted lines correspond to calculations of other authors (reference [21]), while our model levels (the E^+ branch) are represented by dashed lines. In the abscissa we indicate the total angular momentum J .

$x'_{\perp \mu s}, \mu = 0, 1, 2, 3; s = 1, 2$, modulated by an antisymmetric constant tensor $F^{\sigma\tau}$, giving rise to a Poincaré invariant equation of the form

$$\left\{ \sum_{s=1}^2 \Gamma_s [\gamma_s^\mu (p_{\mu s} - \frac{e}{2} \epsilon_{\mu\nu\sigma\tau} x'_{\perp s} F^{\sigma\tau}) + 1] \right\} \psi = 0. \quad (65.1)$$

We shall consider only $F^{\sigma\tau}$ that, in the frame of reference where the center of mass is at rest, i.e., $P_i = 0, i = 1, 2, 3$, reduce to the purely magnetic form

$$F^{ij} = 0, \quad i, j = 1, 2, 3; \quad (65.2a)$$

$$F^{i0} = \frac{1}{2} \mathcal{H}_i, \quad i = 1, 2, 3. \quad (65.2b)$$

An analysis entirely similar to the one that leads from (62.52) to (62.55) allow us to write Eq. (65.1) in the frame of reference where the center of mass is at rest, and where the relation (65.2) holds, in the form

$$\{(\alpha_1 - \alpha_2) \cdot [\mathbf{p} - (e/2)(\mathbf{r} \times \mathcal{H})] + \beta_1 + \beta_2\} \psi = E \psi. \quad (65.3)$$

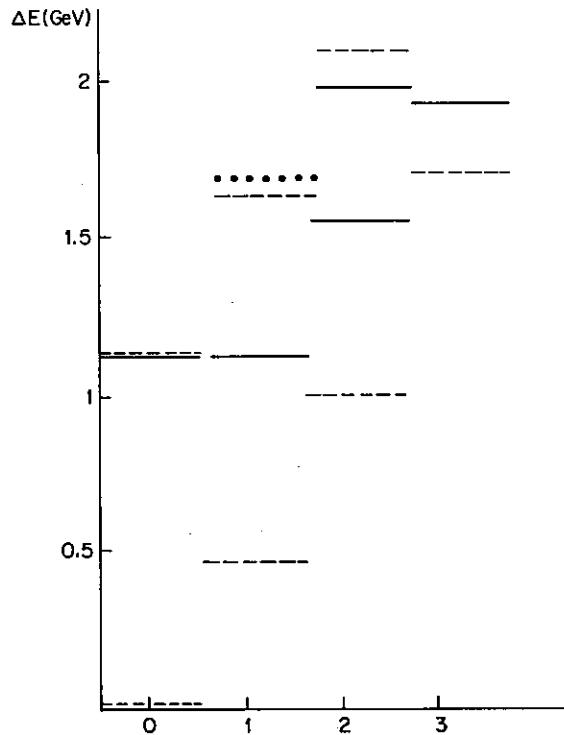


Figure XII.13. The same as XII.12 for isovector mesons, but in this case dashed lines represent levels calculated from the E^- .

We can write Eq. (65.3) as a 4×4 matrix operator using expressions of type (61.12) for the matrices $\alpha_1, \alpha_2, \beta_1, \beta_2$, acting on ψ that is a four-component column vector of the form (61.13). In that case using an analysis similar to the one that takes us from (62.5) to (62.9) and introducing the (ϕ_+, ϕ_-) related to (ψ_{11}, ψ_{22}) by the transformation (61.15) we obtain for the former the equation

$$O \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} \equiv \begin{bmatrix} 4(\mathbf{S} \cdot \mathbf{B})^2 - E^2 & 2E \\ 2E & 4[B^2 - (\mathbf{S} \cdot \mathbf{B})^2] - E^2 \end{bmatrix} \begin{bmatrix} \phi_+ \\ \phi_- \end{bmatrix} = 0, \quad (65.4)$$

where \mathbf{S} is the total spin given by (61.17) and the vector \mathbf{B} is defined by

$$\mathbf{B} \equiv \mathbf{p} - (e/2)(\mathbf{r} \times \mathcal{H}), \quad (65.5)$$

where, as before, $\mathbf{p} = (1/2)(\mathbf{p}_1 - \mathbf{p}_2), \mathbf{r} = (\mathbf{x}_1 - \mathbf{x}_2)$, and \mathcal{H} has the components \mathcal{H}_i in (65.2b).

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As a last step we write (65.4) as two equations, between which we can eliminate ϕ_- , and thus obtain for ϕ_+ , which from now on we denote only as ϕ , the equation

$$\mathcal{O}\phi \equiv \{4E^2 - [4B^2 - 4(\mathbf{S} \cdot \mathbf{B})^2 - E^2][4(\mathbf{S} \cdot \mathbf{B})^2 - E^2]\}\phi = 0. \quad (65.6)$$

We shall proceed to obtain from equation (65.6) the expression for the eigenvalues E of the problem as well as their corresponding eigenfunctions. For this purpose we note that the expression (65.5) of \mathbf{B} is exactly of the same form as the one appearing in the square bracket of equations (60.4,5). Thus if we choose our coordinate x_3 in the direction of the vector \mathcal{H} we obtain for B^2 the expression in the square bracket of (60.6) but without the $e\mathcal{H}\sigma_3$ term. Carrying then a transformation to creation and annihilation operators, as in (60.7,8) we obtain in analogy to (60.9) that

$$B^2 = [e\mathcal{H}(2\eta_+\xi^+ + 1) + p_3^2]. \quad (65.7)$$

On the other hand,

$$\mathbf{B} \cdot \mathbf{S} = \frac{1}{2}B_-S_+ + B_3S_3 + \frac{1}{2}B_+S_-, \quad (65.8)$$

where

$$B_{\pm} = B_1 \pm iB_2, \quad S_{\pm} = S_1 \pm iS_2, \quad (65.9)$$

and from (65.5) and (60.7,8) we have that

$$B_+ = 2i\left(\frac{e\mathcal{H}}{2}\right)^{\frac{1}{2}}\eta_+, \quad B_- = -2i\left(\frac{e\mathcal{H}}{2}\right)^{\frac{1}{2}}\xi^+, \quad (65.10)$$

so that finally

$$\mathbf{S} \cdot \mathbf{B} = i\left(\frac{e\mathcal{H}}{2}\right)^{\frac{1}{2}}[-S_+\xi^+ + S_-\eta_+] + S_3p_3. \quad (65.11)$$

Thus we see that the operator in the curly bracket of (65.6) depends only on η_+ , ξ^+ , p_3 and the components S_{\pm} , S_3 of the total spin. Clearly this operator commutes with

$$\eta_-\xi^-, \quad p_3, \quad S^2 \quad \text{and} \quad J_3 = \eta_+\xi^+ - \eta_-\xi^- + S_3, \quad (65.12)$$

and thus its eigenstates can be given in terms of the kets $|\mu nk\tau\rangle$ of (60.16), only that for spin $s = 0$ the χ_τ is suppressed while, for spin $s = 1$, χ_τ corresponds to this type of spinor where $\tau = 1, 0, -1$, instead of $\pm\frac{1}{2}$ for the one particle case.

If the total spin $s = 0$ the term $\mathbf{S} \cdot \mathbf{B} = 0$ disappears and equation (65.6) becomes

$$E^2[4 + 4e\mathcal{H}(2\eta_+\xi^+ + 1) + 4p_3^2 - E^2]\phi = 0, \quad (65.13)$$

so one of the eigenvalues is $E = 0$ corresponding to an infinitely degenerate state, *i.e.*, a cockroach nest as was discussed in section 61. For the other eigenvalues we apply the square bracket of (65.13) to the states (60.16), where we suppress χ_τ , and use (60.15) with $\tau = 0$ and $n_- \equiv n$, to get

$$E_{\mu nk}^2 = 4 + 4e\mathcal{H}(2\mu + 2n + 1) + 4k^2, \quad (65.14)$$

where

$$n = 0, 1, 2, \dots, \mu = 0, \pm 1, \pm 2, \dots, -\infty \leq k \leq \infty. \quad (65.15)$$

The absence of η_- , ξ^- in the operator of (65.13) indicates again that there is an accidental degeneracy given by a Weyl group.

For the eigenvalues of the energy when the spin $s = 1$ we need the matrix of \mathcal{O} with respect to the states $|\mu nk\tau\rangle$ of (60.16) where $\tau = 1, 0, -1$. Because of the integrals of motion (65.12) this matrix is diagonal in μ , n , k and only τ can vary in bra and ket, so that we get a 3×3 numerical matrix. To determine it we only need to use the well known results

$$\eta_+ | n_+ \rangle = (n_+ + 1)^{\frac{1}{2}} | n_+ + 1 \rangle, \quad \xi^+ | n_+ \rangle = n_+^{\frac{1}{2}} | n_+ - 1 \rangle, \quad (65.16)$$

$$S_{\pm}\chi_\tau = [(1 \mp \tau)(2 \pm \tau)]^{\frac{1}{2}}\chi_{\tau \pm 1}, \quad S_3\chi_\tau = \tau\chi_\tau, \quad (65.17)$$

to get for the operator in the curly bracket of (65.6) the matrix expression

$$\begin{pmatrix} \mathcal{A} & ik(\frac{\delta}{e\mathcal{H}})^{\frac{1}{2}} & 2[\delta(\delta + 1)]^{\frac{1}{2}} \\ ik(\frac{\delta}{e\mathcal{H}})^{\frac{1}{2}} & \mathcal{B} & -ik(\frac{\delta+1}{e\mathcal{H}})^{\frac{1}{2}} \\ -2[\delta(\delta + 1)]^{\frac{1}{2}} & -ik(\frac{\delta+1}{e\mathcal{H}})^{\frac{1}{2}} & \mathcal{C} \end{pmatrix}, \quad (65.18a)$$

where

$$\mathcal{A} = [\epsilon^2 - \epsilon(2\delta - 1 + \frac{k^2}{e\mathcal{H}} + \frac{1}{e\mathcal{H}}) - \frac{k^2}{e\mathcal{H}} - 2\delta], \quad (65.18b)$$

$$\mathcal{B} = \epsilon^2 - \epsilon(2\delta + \frac{k^2}{e\mathcal{H}} + \frac{1}{e\mathcal{H}} + 1), \quad (65.18c)$$

$$\mathcal{C} = [\epsilon^2 - \epsilon(2\delta + \frac{k^2}{e\mathcal{H}} + \frac{1}{e\mathcal{H}} + 3) + 2\delta + \frac{k^2}{e\mathcal{H}} + 2], \quad (65.18d)$$

and

$$\delta \equiv \mu + n, \quad \epsilon \equiv (\frac{E^2}{4e\mathcal{H}}). \quad (65.19)$$

The determinant of this matrix gives the secular equation, of sixth degree in ϵ , that determines the energy levels E for fixed μ, n, k , and thus the problem has been reduced to a purely algebraic one.

We shall discuss, in particular, the case when $k = 0$, i.e., when there is no motion in the direction of the vector \mathcal{H} , when the secular equation takes the form

$$\begin{aligned} & \{\epsilon^2 - \epsilon[2\delta + e^{-1}\mathcal{H}^{-1} + 1]\}\{4\delta(\delta + 1) \\ & + [\epsilon^2 - \epsilon(2\delta - 1 + e^{-1}\mathcal{H}^{-1}) - 2\delta] \\ & \times [\epsilon^2 - \epsilon(2\delta + e^{-1}\mathcal{H}^{-1} + 3) + 2\delta + 2]\} = 0. \end{aligned} \quad (65.20)$$

From equation (65.20) it follows that there are the roots

$$E^2 = 0, \quad (65.21)$$

$$E^2 = 4 + 4e\mathcal{H}[2(\mu + n) + 1], \quad (65.22)$$

while the others satisfy the fourth degree equation in the ϵ 's of the form

$$\begin{aligned} & \{4\delta(\delta + 1) + [\epsilon^2 - \epsilon(2\delta - 1 + e^{-1}\mathcal{H}^{-1}) - 2\delta] \\ & \times [\epsilon^2 - \epsilon(2\delta + e^{-1}\mathcal{H}^{-1} + 3) + 2\delta + 2]\} = 0. \end{aligned} \quad (65.23)$$

Again $E = 0$ of (65.21) corresponds to a cockroach nest of section 61, while the E of (65.22) has an accidental degeneracy associated with a Weyl algebra whose generators are $\eta_-, \xi^-, 1$. The energy levels obtained by solving (65.23) have also an accidental degeneracy of the same type as the ϵ will depend only on $\delta = \mu + n$, with the values of μ and n given in (65.15).

The determination of the energy levels has thus been reduced to one of algebraic computation, which could be carried out for all the cases of interest. We conclude by indicating the possible conceptual or physical implications of the present analysis.

We have discussed an exactly soluble relativistic two-body problem in which the interaction is linear in the relative coordinate, but modulated by a constant antisymmetric tensor.

Our first objective will be to compare the solutions in this section with those when the interaction was of a Dirac oscillator type, i.e., instead of equation (65.1) we will consider equation (62.52)

As was discussed in (62.13), the commuting integrals of motion in the two-body Dirac oscillator problem turn out to be

$$\hat{N} = \boldsymbol{\eta} \cdot \boldsymbol{\xi}, \quad J^2 = [-i(\boldsymbol{\eta} \times \boldsymbol{\xi}) + \mathbf{S}]^2, \quad J_z, \quad S^2, \quad \mathcal{P}, \quad (65.24)$$

where $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ are now three-dimensional creation and annihilation operators, and \mathcal{P} is the parity.

The basic kets are now no longer $|n_+n_-k\tau\rangle$ or $|\mu nk\tau\rangle$ of (60.10) and (60.16), respectively, with $\tau = 1, 0, -1$ but

$$|N(\ell, s)jm\rangle, \quad (65.25)$$

where N is the total number of quanta, ℓ the orbital and j the total angular momentum and m its projection, while $s = 0, 1$ is the total spin.

Thus, our present problem is soluble in a cylindrical basis with spin, where in the direction of \mathcal{H} the particle is free, and in the plane perpendicular to \mathcal{H} it is an harmonic oscillator, while the example with Dirac oscillator interaction is soluble in an oscillator basis with spin in spherical coordinates. Note also that the two particles problem with a Dirac oscillator interaction when $B = \beta_1\beta_2$ has an accidental degeneracy *only* for the case of parity $(-1)^j$, and explained by an $o(4)$ symmetry Lie algebra. On the other hand our present problem has *always* an accidental degeneracy explained by the Weyl Lie algebra whose generators are $\eta_-, \xi^-, 1$.

We would like also to point that, at least for the case when the spin $s = 0$, our problem is identical to that of a Klein-Gordon particle in a constant electromagnetic field, whose Poincaré invariant equation is

$$[(p_\mu - eA_\mu)(p^\mu - eA^\mu) + 1]\psi = 0, \quad (65.26)$$

with A_μ being the four-vector potential. Choosing a frame of reference in which A_μ is purely magnetic, i.e.,

$$A_0 = 0, \quad A = \frac{1}{2}(\mathbf{r} \times \mathcal{H}), \quad (65.27)$$

and denoting, as before, the energy by E , we have

$$\left[p - \frac{e}{2}(\mathbf{r} \times \mathcal{H}) \right]^2 \psi = (E^2 - 1)\psi, \quad (65.28)$$

and thus, from the relations (60.15), (65.5) and (65.7) we get

$$E_{\mu nk}^2 = 1 + e\mathcal{H}(2\mu + 2n + 1) + k^2, \quad (65.29)$$

which coincides with (65.14) except for the coefficient 4, associated with the fact that in (65.29) we are dealing with a single particle of mass 1, while (65.14) corresponds to two particles of this mass whose square is 4.

66 Formulation of the Oscillator Problem Through Two Independent, But Constrained, Relativistic Equations

In all the previous analysis of the relativistic two-body problem, we started with a single Poincaré invariant equation for the two particles. Its first appearance was in connection with two free particles in section 61, though in sections 64 to 65 it was obtained when the two bodies had different types of oscillator interactions. In this section we shall follow a procedure more familiar in the literature [3], where we start with independent relativistic equations for each of the two particles, containing a Poincaré invariant interaction. We furthermore impose a constraint on these equations so they are compatible and allow us, in the frame of reference where the center of mass is at rest, to eliminate the variables that have no physical significance, such as the relative time of the two particles, *i.e.*, $x_{01} - x_{02}$.

As in the previous sections we shall, for simplicity, deal only with two particles of equal mass and continue to use the units $\hbar = m = c = 1$. We shall discuss the systems of two scalar particles, a scalar and a spinor particle, and two spinor particles.

a) The case of two scalar particles

In this case we need to find a wave function ψ satisfying a system of two equations of the form

$$(p_1^\mu p_{\mu 1} + 1 + V_1)\psi = 0, \quad (66.1a)$$

$$(p_2^\mu p_{\mu 2} + 1 + V_2)\psi = 0, \quad (66.1b)$$

where V_1 and V_2 are, so far, arbitrary functions of $x_{\mu s}$ and $p_{\mu s}$, $\mu = 0, 1, 2, 3$, $s = 1, 2$, so long as they are invariant under the transformations of the Poincaré group.

If we write $p_{\mu 1}$ and $p_{\mu 2}$, in terms of the total P_μ and relative p_μ momentum four vectors, *i.e.*,

$$p_{\mu 1} = \frac{1}{2}P_\mu + p_\mu, \quad (66.2a)$$

$$p_{\mu 2} = \frac{1}{2}P_\mu - p_\mu, \quad (66.2b)$$

and subtract the two equations in (66.1) we arrive at the relation

$$2p_\mu P^\mu \psi = (V_2 - V_1)\psi. \quad (66.3)$$

Now the constraint we wish to impose is that the right hand vanishes, *i.e.*,

$$V_1 = V_2 \equiv V, \quad (66.4)$$

because then the equation become

$$p_\mu P^\mu \psi = 0, \quad (66.5)$$

and in the reference frame where the center of mass is at rest, *i.e.*, $P_i = 0$, $i = 1, 2, 3$, and P^0 has the definite eigenvalue E of the total energy, Eq. (66.5) becomes

$$-iE(\partial\psi/\partial x^0) = 0, \quad (66.6)$$

and thus the wave function will be independent of the relative time x^0 .

Adding the two equations, in the frame of reference mentioned, gives us now, when Eq. (66.6) is taken into account, that

$$(2p \cdot p - \frac{1}{2}E^2 + 2 + 2V)\psi = 0. \quad (66.7)$$

For an oscillator potential we can take V as

$$V = \omega^2(x_{\perp\mu}x_\perp^\mu) = \omega^2 r^2, \quad (66.8)$$

where $x_{\perp\mu}$ is the transverse part (62.50) of the relative four vector $x_{1\mu} - x_{2\mu}$ and, in the reference frame where the center of mass is at rest, it becomes r^2 as indicated in Eq. (66.8). Thus we now have the equation

$$4(-\nabla^2 + \omega^2 r^2)\psi = (E^2 - 4)\psi, \quad (66.9)$$

entirely similar to (58.11) and whose solutions are given by (58.12), while the spectrum becomes

$$E^2 = 4 + 8\omega\left(N + \frac{3}{2}\right). \quad (66.10)$$

This elementary example is discussed here just to show the type of constraint (66.5,6) that has to be imposed if we want to eliminate the unphysical degree of freedom of relative time x^0 .

b) The case of a scalar and spinorial particles

The equations we have now are

$$(\gamma^\mu p_{\mu 1} + 1 + V_1)\psi = 0, \quad (66.11a)$$

$$(p_{2\mu} p_2^\mu + 1 + V_2)\psi = 0. \quad (66.11b)$$

We multiply Eq. (66.11a) by $(-\gamma^\mu p_{\mu 1} + 1)$ and we get from (59.25a) the expression

$$[(p_{1\mu} p_1^\mu + 1) - (\gamma^\mu p_{\mu 1} - 1)V_1]\psi = 0. \quad (66.12)$$

Subtracting (66.11b) from (66.12) we obtain, with the help of (66.2), that

$$2P^\mu p_\mu \psi = [V_2 + (\gamma^\mu p_{\mu 1} - 1)V_1]\psi. \quad (66.13)$$

Again we would like the constraint (66.5) to hold as it will eliminate the unphysical x^0 and thus we are led to the conclusion that V_2 is a function of V_1 , *i.e.*,

$$V_2 = -(\gamma^\mu p_{\mu 1} - 1)V_1, \quad (66.14)$$

though V_1 can be any function of $\gamma^\mu, x_{\mu s}, p_{\mu s}, s = 1, 2$ so long as it is Poincaré invariant. If we choose

$$V_1 = -i\omega(\gamma^\mu x_{\perp\mu})(\gamma^\nu u_\nu), \quad (66.15)$$

with $x_{\perp\mu}$ being the transversal part (62.50) of $x_{\mu 1} - x_{\mu 2}$, and u_μ given by (62.53) we see that, in the frame of reference where the center of mass is at rest, we get that Eq. (66.11a) becomes

$$[\alpha \cdot (p - i\omega r\beta) + \beta]\psi = (E/2)\psi, \quad (66.16)$$

where we made use of Eq. (66.2) and the fact that $P_i = 0, i = 1, 2, 3$, $P^0 = E$.

Equation (66.16) happens to be exactly the one particle Dirac oscillator discussed in section 59, except that E is replaced by $(E/2)$, and thus all the results derived there can be applied to it. Again the example was mainly discussed to show that the approach we follow here allows us to derive results with which we are already familiar.

c) The case of two spinorial particles

We shall consider the single free particle Dirac equations in the form used by Crater and van Alstein [22], *i.e.*,

$$[\gamma_{5s}(\gamma_s \cdot p_s + 1)]\psi = 0, \quad s = 1, 2, \quad (66.17)$$

where we replaced indices $\mu = 0, 1, 2, 3$ by a dot, but when passing to the system with interaction we follow the notation of Sazdjian [23], *i.e.*,

$$[\gamma_{51}(\gamma_1 \cdot p_1 + 1) + V_1]\psi = 0, \quad (66.18a)$$

$$[\gamma_{52}(\gamma_2 \cdot p_2 + 1) + V_2]\psi = 0, \quad (66.18b)$$

and the first problem is to prove the compatibility of the system. This is achieved [22,23] by multiplying the first equation by $\gamma_{51}(\gamma_1 \cdot p_1 + 1)$ and the second by $\gamma_{52}(\gamma_2 \cdot p_2 + 1)$ and subtracting, so from the properties (59.25a) of the γ matrices and the relations (66.2) we arrive at the equation

$$[2p \cdot P + \gamma_{51}(\gamma_1 \cdot p_1 + 1)V_1 - \gamma_{52}(\gamma_2 \cdot p_2 + 1)V_2]\psi = 0. \quad (66.19)$$

Thus, as we wish to impose the constraint $P \cdot p\psi = 0$ of (66.5), we see that V_1, V_2 are related by the expression

$$\gamma_{51}(\gamma_1 \cdot p_1 + 1)V_1\psi = \gamma_{52}(\gamma_2 \cdot p_2 + 1)V_2\psi, \quad (66.20)$$

which implies that

$$V_1 = \gamma_{52}(\gamma_2 \cdot p_2 + 1)V, \quad V_2 = \gamma_{51}(\gamma_1 \cdot p_1 + 1)V, \quad (66.21)$$

where V has to be a Poincaré invariant so that Eqs. (66.18) have also this property. The simplest way to achieve this behavior is to use the transverse relative coordinate and call the scalar formed from its contraction with itself as

$$\rho^2 = x_{\perp}^\mu x_{\perp\mu}, \quad (66.22)$$

so we shall assume that V is only a function of ρ .

We now have the set of two compatible equations

$$\left\{ \gamma_{51}(\gamma_1 \cdot p_1 + 1) + \gamma_{52}(\gamma_2 \cdot p_2 + 1)V \right\}\psi = 0, \quad (66.23a)$$

$$\left\{ \gamma_{52}(\gamma_2 \cdot p_2 + 1) + \gamma_{51}(\gamma_1 \cdot p_1 + 1)V \right\}\psi = 0. \quad (66.23b)$$

If in (66.23a) we pass V to the left of the operator $\gamma_{52}(\gamma_2 \cdot p_2 + 1)$, adding a term from the commutation that gives a derivative of V with respect to x_2^μ , and then use (66.23b) to substitute the term $V\gamma_{52}(\gamma_2 \cdot p_2 + 1)$ appearing in (66.23a) we get

$$\left\{ \gamma_{51}(\gamma_1 \cdot p_1 + 1) - V\gamma_{51}(\gamma_1 \cdot p_1 + 1)V - i\gamma_{52}(\gamma_2 \cdot \partial_2 V) \right\}\psi = 0, \quad (66.24)$$

where $\gamma_2 \cdot \partial_2 = \gamma_2^\mu \partial/\partial x_2^\mu$.

Finally moving all the terms V in (66.24) to the left hand side, and multiplying the resulting equation by $\gamma_{51}(1 - V^2)^{-1}$ we get

$$\left\{ (\gamma_1 \cdot p_1 + 1) + (1 - V^2)^{-1}[-i\gamma_{51}\gamma_{52}(\gamma_2 \cdot \partial_2 V) + iV(\gamma_1 \cdot \partial_1 V)] \right\}\psi = 0, \quad (66.25a)$$

Carrying out a similar analysis, but now starting from (66.23b), we obtain in turn

$$\left\{ (\gamma_2 \cdot p_2 + 1) + (1 - V^2)^{-1} [-i\gamma_{51}\gamma_{52}(\gamma_1 \cdot \partial_1 V) + iV(\gamma_2 \cdot \partial_2 V)] \right\} \psi = 0. \quad (66.25b)$$

We now make a change in our function ψ through the relation

$$\psi = (1 - V^2)^{-1/2} \phi \quad (66.26)$$

and consider the replacements of p_1 and p_2 indicated in (66.2), using also the fact that as V is a function of r , so

$$(\partial V / \partial x_s^\mu) = (\partial V / \partial \rho)(\partial \rho / \partial x_s^\mu) \equiv \dot{V}(x'_{\mu \perp} / \rho)(-1)^{s+1}, \quad (66.27)$$

we obtain finally that Eq. (66.25) reduces to

$$\left\{ (\gamma_1 \cdot p + \frac{1}{2}\gamma_1 \cdot P + 1) + (1 - V^2)^{-1} \times \dot{V}[i\gamma_{51}\gamma_{52}(\gamma_2 \cdot x'_{\perp})\rho^{-1}] \right\} \phi = 0, \quad (66.28a)$$

$$\left\{ (-\gamma_2 \cdot p + \frac{1}{2}\gamma_2 \cdot P + 1) + (1 - V^2)^{-1} \times \dot{V}[-i\gamma_{51}\gamma_{52}(\gamma_1 \cdot x'_{\perp})\rho^{-1}] \right\} \phi = 0. \quad (66.28b)$$

Passing now to the center of mass frame where $\gamma_1 \cdot P = \beta_1 P_0 = -\beta_1 E$, $\gamma_2 \cdot P = \beta_2 P_0 = -\beta_2 E$, and multiplying (66.28a) by β_1 , and (66.28b) by β_2 , and remembering that ϕ does not depend on x_0 , as well as the relations for the three-component vectors

$$\gamma_1 = \beta_1 \alpha_1, \gamma_2 = \beta_2 \alpha_2, \quad (66.29)$$

we see that by adding the two equations (66.28) modified in this fashion we finally obtain

$$\left\{ (\alpha_1 - \alpha_2) \cdot p + \beta_1 + \beta_2 + \dot{V}[r(1 - V^2)]^{-1} \times [i\beta_1\gamma_{51}\gamma_{52}(\gamma_2 \cdot r) - i\beta_2\gamma_{51}\gamma_{52}(\gamma_1 \cdot r)] \right\} \phi = E\phi, \quad (66.30)$$

where p, r are the relative spatial three-component vectors of momentum and position, while V is a function of the magnitude r and $\dot{V} = (dV/dr)$.

It is now a question of selecting the form of the function $V(r)$. Following Sazdjian [23] and Crater and van Alstine [22], we write V as an hyperbolic tangent but, for our future purposes, the argument is taken as $(\omega r^2/4)$, i.e.,

$$V(r) = \tanh(\omega r^2/4). \quad (66.31)$$

We see then that Eq. (66.30) becomes

$$\left\{ (\alpha_1 - \alpha_2) \cdot (p - i\frac{\omega}{2}r\beta_1\beta_2\gamma_{51}\gamma_{52}) + \beta_1 + \beta_2 \right\} \phi = E\phi, \quad (66.32)$$

and so it has exactly the form of (62.4) when $B = \beta_1\beta_2\gamma_{51}\gamma_{52}$, and its eigenvalues and eigenfunctions were discussed in section 62 between Eqs. (62.37) and (62.49). Again the objective of this section was to show that the analysis of the Dirac equations with a constrained interaction, leads to exactly one of the results obtained with a single Poincaré invariant equation.

We note that our Eq. (66.32) was derived from the sum of the two equations in (66.28), when written in the frame of reference where the center of mass is at rest and appropriately modified. What happens when, with the modifications we considered, we look at the difference between these two equations, again in the frame of reference where the center mass is at rest? We note that E no longer appears in the resulting equations and, again following an analysis very similar to the one that led from (62.37) to (62.38), we obtain that now ϕ_+, ϕ_- must obey the equations

$$\{[\sigma_1 - \sigma_2] \cdot \eta][(\sigma_1 + \sigma_2) \cdot \eta]\} \phi_- = 0, \quad (66.33a)$$

$$\{[\sigma_1 - \sigma_2] \cdot \xi][(\sigma_1 + \sigma_2) \cdot \xi]\} \phi_+ = 0. \quad (66.33b)$$

It is easy to show though that, using the relation

$$\sigma_i \sigma_j = \delta_{ij} + i\epsilon_{ijk} \sigma_k \quad (66.34)$$

for both Pauli spin matrices σ_1 and σ_2 , the curly brackets vanish identically and thus they do not impose any further restriction on ϕ_+, ϕ_- as we could have expected from the compatible character of the two equations (66.18) required from the beginning.

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Chapter XIII

The n -Body Relativistic Oscillator

In the previous chapters we discussed different examples of one and two-body relativistic systems with harmonic oscillator interactions. We stress again that we dealt only with relativistic quantum mechanics of the systems mentioned but not with relativistic quantum field theory, and the same restriction will apply here when we pass to the n -body problem. While our analysis will actually be valid for any number of particles, the specific examples we shall discuss in detail concern three scalar or three spinor-like particles in their center of mass frame, with the latter being applied to three quarks, to get a mass formula for non-strange baryons. We shall start with the problem of n free scalar nonrelativistic particles to show how we can pass to the system where they have an oscillator interaction and this procedure will later be generalized to the relativistic case.

67 The Nonrelativistic Problem for n -Free Scalar Particles and Its Extension to a System with Harmonic Oscillator Interactions

Let us first start with a system of n free nonrelativistic particles of the same mass m , and take units

$$\hbar = m = c = 1, \quad (67.1)$$

where the velocity of light will appear only in the next section, but we want to start from the beginning with units in which everything is dimensionless.

The classical total energy is then

$$E = (1/2) \sum_{s=1}^n \mathbf{p}_s \cdot \mathbf{p}_s, \quad (67.2)$$

where \mathbf{p}_s are the three-dimensional classical momentum vectors of particle s .

From the beginning we would like to work in the center of mass frame, because our interest will be the internal energy of the system and not the contribution from its center of mass motion. The best way to achieve this is to pass to Jacobi momenta [1] defined by the orthogonal transformation

$$\dot{\mathbf{p}}_s = [s(s+1)]^{-\frac{1}{2}} \left[\sum_{t=1}^s \mathbf{p}_t - s\mathbf{p}_{s+1} \right], \quad s = 1, 2, \dots, n-1, \quad (67.3a)$$

$$\dot{\mathbf{p}}_n = n^{-\frac{1}{2}} \sum_{s=1}^n \mathbf{p}_s. \quad (67.3b)$$

Clearly $\dot{\mathbf{p}}_n$ is proportional to the total momentum and in the center of mass system it will vanish, so Eq. (67.2) reduces to

$$E = \frac{1}{2} \sum_{s=1}^{n-1} \dot{\mathbf{p}}_s \cdot \dot{\mathbf{p}}_s. \quad (67.4)$$

The Schroedinger equations corresponding to (67.4) is obtained when we replace $\dot{\mathbf{p}}_s$ by the operator

$$\hat{\mathbf{p}}_s = \frac{1}{i} \frac{\partial}{\partial \dot{\mathbf{x}}_s}, \quad (67.5)$$

with $\dot{\mathbf{x}}_s$ being the corresponding Jacobi coordinate vector. As the $\dot{\mathbf{p}}_s$ are hermitian operators we can also write the Schroedinger equation as

$$\frac{1}{2} \sum_{s=1}^{n-1} \left(\hat{\mathbf{p}}_s^\dagger \cdot \hat{\mathbf{p}}_s \right) \psi = E\psi. \quad (67.6)$$

We can easily transform this into an hermitian oscillator operator equation if we make the replacement

$$\dot{\mathbf{p}}_s \rightarrow \dot{\mathbf{p}}_s - i\omega \dot{\mathbf{x}}_s, \quad (67.7a)$$

$$\hat{\mathbf{p}}_s^\dagger \rightarrow \hat{\mathbf{p}}_s + i\omega \dot{\mathbf{x}}_s, \quad (67.7b)$$

where the second equation follows from the first as both $\dot{\mathbf{p}}_s$ and $\dot{\mathbf{x}}_s$ are hermitian operators.

Thus we now get a Schroedinger equation of the form

$$\left\{ \frac{1}{2} \sum_{s=1}^{n-1} \left[\dot{\mathbf{p}}_s^2 + \omega^2 \dot{\mathbf{x}}_s^2 \right] - (3/2)\omega(n-1) \right\} \psi = E\psi, \quad (67.8)$$

whose eigenvalue for the energy E will be

$$E = \omega N, \quad (67.9)$$

with N being the total number of quanta, *i.e.*,

$$N = \sum_{s=1}^{n-1} N_s. \quad (67.10)$$

The previous analysis is standard except for the fact that we start from a system of n free particles. Furthermore our notation in terms of three vectors and Jacobi coordinates avoids the worry about the Galilean invariance of the whole procedure. We will now consider a similar set of steps for a relativistic problem.

68 The System of Three Relativistic Scalar Particles with Oscillator Interactions

Rather than discuss the system of n relativistic particles, we shall restrict ourselves to $n = 3$, as we will see that the case is general enough, with only the algebraic steps becoming more complicated as n increases.

In our units the total energy for a system of three free relativistic particles can be written as

$$E = \pm \Pi_1 \pm \Pi_2 \pm \Pi_3, \quad (68.1)$$

where Π_s , $s = 1, 2, 3$, is defined as

$$\Pi_s \equiv (p_s^2 + 1)^{\frac{1}{2}}. \quad (68.2)$$

It is very important to note that, in our units, Einstein relation is $E^2 = p^2 + 1$, and when reduced to the E itself gives both the square root in (68.2) and the \pm signs in (68.1).

Obviously we can not get a Schroedinger equation from relation (68.1), but we can take $\pm \Pi_3$ to the right hand side and square both sides. Then

we can square again and again appropriately, and we easily arrive at the fact that (68.1) becomes an eight degree equation in E (actually of fourth degree in E^2) of the form

$$\begin{aligned}\Phi(E^2, \Pi_s^2) &\equiv E^8 - 4AE^6 + (4A^2 + 2B)E^4 \\ &\quad - (4C^2 + 4AB)E^2 + B^2 = 0,\end{aligned}\quad (68.3)$$

where A, B, C are functions of Π_s^2 , $s = 1, 2, 3$, given by

$$A \equiv \Pi_1^2 + \Pi_2^2 + \Pi_3^2, \quad (68.4a)$$

$$\begin{aligned}B &\equiv \Pi_1^4 + \Pi_2^4 + \Pi_3^4 - \Pi_1^2\Pi_2^2 - \Pi_2^2\Pi_3^2 \\ &\quad - \Pi_1^2\Pi_3^2 - \Pi_2^2\Pi_1^2 - \Pi_3^2\Pi_2^2 - \Pi_1^2\Pi_1^2 \quad \approx\end{aligned}\quad (68.4b)$$

$$\begin{aligned}C^2 &\equiv \frac{8}{3}(\Pi_1^2\Pi_2^2\Pi_3^2 + \Pi_2^2\Pi_1^2\Pi_3^2 + \Pi_3^2\Pi_1^2\Pi_2^2 + \Pi_1^2\Pi_3^2\Pi_2^2 \\ &\quad + \Pi_3^2\Pi_2^2\Pi_1^2 + \Pi_2^2\Pi_3^2\Pi_1^2).\end{aligned}\quad (68.4c)$$

Note that as we are working with classical observables that commute we could express A, B, C^2 of (68.4) in a much more compact form. We prefer though to write them in an explicitly invariant way under permutation of the indices $s = 1, 2, 3$, as later Π_s^2 will be replaced by operators that do not commute.

Now we can write an equation that does not have E as an eigenvalue, but in which it appears as a parameter, if we replace p_s by $-i\partial/\partial x_s$, as in (67.5), so that Π_s^2 become the operators

$$\hat{\Pi}_s^2 = (-\nabla_s^2 + 1), \quad (68.5)$$

and we get

$$\Phi(E^2, \hat{\Pi}_s^2)\psi = 0. \quad (68.6)$$

Thus far we have obtained nothing useful because p_1, p_2 and p_3 , considered as operators of the form (67.5), commute with the operator Φ and are integrals of motion, so that ψ can be written as

$$\psi = \exp[i(p_1 \cdot x_1 + p_2 \cdot x_2 + p_3 \cdot x_3)], \quad (68.7)$$

where now p_1, p_2 and p_3 are ordinary numbers and we are returned to equation (68.3) whose eight roots for the energy E are obviously given by (68.1) with all the possible combination of the signs \pm .

Before proceeding further, along the lines of the previous section, we again remark that we would like to work in the center of mass frame, as our interest is restricted to the internal energy of the system. Thus we go,

as in section 67, to the Jacobi momenta \dot{p}_s , $s = 1, 2, 3$, which from (67.3) are given now by the matrix relation

$$\begin{pmatrix} \dot{p}_1 \\ \dot{p}_2 \\ \dot{p}_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}. \quad (68.8)$$

As the matrix is orthogonal, transposing it we get p_s in terms of \dot{p}_s , and as we want to be in the center of mass frame $\dot{p}_3 = 0$, so we get finally

$$p_1 = \frac{1}{\sqrt{2}}\dot{p}_1 + \frac{1}{\sqrt{6}}\dot{p}_2, \quad p_2 = -\frac{1}{\sqrt{2}}\dot{p}_1 + \frac{1}{\sqrt{6}}\dot{p}_2, \quad p_3 = -\sqrt{\frac{2}{3}}\dot{p}_2. \quad (68.9)$$

As Eq. (68.6) contains only powers of $\hat{\Pi}_s^2$, $s = 1, 2, 3$, we can write the latter using the hermitian property of \dot{p}_s , now considered as operators of the type (67.5), as

$$\hat{\Pi}_1^2 = \frac{1}{2}\dot{p}_1^\dagger \cdot \dot{p}_1 + \frac{1}{6}\dot{p}_2^\dagger \cdot \dot{p}_2 + \frac{1}{2\sqrt{3}}(\dot{p}_1^\dagger \cdot \dot{p}_2 + \dot{p}_2^\dagger \cdot \dot{p}_1) + 1, \quad (68.10a)$$

$$\hat{\Pi}_2^2 = \frac{1}{2}\dot{p}_1^\dagger \cdot \dot{p}_1 + \frac{1}{6}\dot{p}_2^\dagger \cdot \dot{p}_2 - \frac{1}{2\sqrt{3}}(\dot{p}_1^\dagger \cdot \dot{p}_2 + \dot{p}_2^\dagger \cdot \dot{p}_1) + 1, \quad (68.10b)$$

$$\hat{\Pi}_3^2 = \frac{2}{3}\dot{p}_2^\dagger \cdot \dot{p}_2 + 1. \quad (68.10c)$$

The interesting point is to introduce the oscillator interaction, exactly as in the replacement we made in (67.7) in the nonrelativistic problem. For notational purposes we introduce the creation and annihilation operators

$$\eta_s \equiv \frac{1}{\sqrt{2}}(\omega^{\frac{1}{2}}\dot{x}_s - i\omega^{-\frac{1}{2}}\dot{p}_s), \quad s = 1, 2, \quad (68.11a)$$

$$\xi_s \equiv \frac{1}{\sqrt{2}}(\omega^{\frac{1}{2}}\dot{x}_s + i\omega^{-\frac{1}{2}}\dot{p}_s), \quad s = 1, 2, \quad (68.11b)$$

so that relations (67.7) can be written as

$$\dot{p}_s \rightarrow -i\omega^{\frac{1}{2}}\sqrt{2}\xi_s, \quad (68.12a)$$

$$\dot{p}_s^\dagger \rightarrow i\omega^{\frac{1}{2}}\sqrt{2}\eta_s. \quad (68.12b)$$

Under this replacement the $\hat{\Pi}_s^2$ operators become then

$$\hat{\Pi}_1^2 = \omega[\dot{C}_{11} + \frac{1}{3}\dot{C}_{22} + \frac{1}{\sqrt{3}}(\dot{C}_{12} + \dot{C}_{21})] + 1, \quad (68.13a)$$

$$\hat{\Pi}_2^2 = \omega[\dot{C}_{11} + \frac{1}{3}\dot{C}_{22} - \frac{1}{\sqrt{3}}(\dot{C}_{12} + \dot{C}_{21})] + 1, \quad (68.13b)$$

$$\hat{\Pi}_3^2 = \frac{4}{3}\omega\dot{C}_{22} + 1, \quad (68.13c)$$

where the operator \dot{C}_{st} , $s, t = 1, 2$, are defined by

$$\dot{C}_{st} = \dot{\eta}_s \cdot \dot{\xi}_t. \quad (68.14)$$

From the fact that

$$[\dot{\xi}_{it}, \dot{\eta}_{js}] = \delta_{ij}\delta_{st}; \quad i, j = 1, 2, 3; \quad s = 1, 2, \quad (68.15)$$

we have the commutation relations

$$[\dot{C}_{st}, \dot{C}_{s't'}] = \dot{C}_{st'}\delta_{s't} - \dot{C}_{s't}\delta_{st'}, \quad (68.16)$$

and thus they are generators [2] of a U(2) group. Therefore the operators $\hat{\Pi}_1^2$, $\hat{\Pi}_2^2$ and $\hat{\Pi}_3^2$, appearing in Eq. (68.6), are linear functions of the generators of this group.

To obtain from Eq. (68.6,13) the eigenvalues of the energy for this relativistic oscillator problem we can proceed as follows: First we note that the first order Casimir operator of U(2) group is

$$\hat{N} = \dot{C}_{11} + \dot{C}_{22}, \quad (68.17)$$

and that it has an SU(2) subgroup whose generators are

$$\hat{F}_+ \equiv \dot{C}_{12}, \quad (68.18a)$$

$$\hat{F}_o \equiv (\frac{1}{2})(\dot{C}_{11} - \dot{C}_{22}), \quad (68.18b)$$

$$\hat{F}_- \equiv \dot{C}_{21}, \quad (68.18c)$$

with a corresponding Casimir operator of the form

$$\hat{F}^2 \equiv \hat{F}_-\hat{F}_+ + \hat{F}_o(\hat{F}_o + 1). \quad (68.19)$$

By definition, \hat{N} and \hat{F}^2 commute with all \dot{C}_{st} and among themselves, so from (68.13), they will be integrals of motion of the operator $\Phi(E^2, \hat{\Pi}_s^2)$. Thus the eigenstates of Eq. (68.6) can be characterized by the eigenvalues of \hat{N} , \hat{F}^2 which we denote respectively by

$$N, \quad \mathcal{F}(\mathcal{F} + 1), \quad (68.20)$$

with \mathcal{F} taking the values $(N/2)$ and $(N/2) - 1$, down to $1/2$ or 0 depending on whether N is odd or even.

Another operator that commutes with \hat{N} and \hat{F}^2 is obviously \hat{F}_o and we shall designate its eigenvalue by

$$\nu = \mathcal{F}, \mathcal{F} - 1, \dots, -\mathcal{F}, \quad (68.21)$$

so the eigenstates associated with \hat{N} , \hat{F}^2 and \hat{F}_o could be represented by the ket

$$|N\mathcal{F}\nu\rangle, \quad (68.22)$$

and the solution ψ of Eq. (68.6) is necessarily a linear combination of these kets, *i.e.*,

$$\psi = \sum_{\nu=-\mathcal{F}}^{\mathcal{F}} a_{\nu} |N\mathcal{F}\nu\rangle, \quad (68.23)$$

as \hat{N} and \hat{F}^2 are integrals of motion.

To obtain the eigenvalues of the internal energy E as function of N and \mathcal{F} we need first to consider the matrix elements of the operator Φ of (68.6) in the basis (68.22), *i.e.*,

$$\langle N\mathcal{F}\nu' | \Phi(E^2, \hat{\Pi}_s^2) | N\mathcal{F}\nu \rangle. \quad (68.24)$$

These elements can be obtained straightforwardly as from (68.13,17,18) we have

$$\hat{\Pi}_1^2 = 1 + \omega[(2/3)(\hat{N} + \hat{F}_o) + (1/\sqrt{3})(\hat{F}_+ + \hat{F}_-)], \quad (68.25a)$$

$$\hat{\Pi}_2^2 = 1 + \omega[(2/3)(\hat{N} + \hat{F}_o) - (1/\sqrt{3})(\hat{F}_+ + \hat{F}_-)], \quad (68.25b)$$

$$\hat{\Pi}_3^2 = 1 + \omega[(2/3)(\hat{N} - 2\hat{F}_o)], \quad (68.25c)$$

and besides we have the well known angular momentum relations which, in the language used here for the SU(2) group, are

$$\hat{F}_{\pm}|N\mathcal{F}\nu\rangle = [(\mathcal{F} \mp \nu)(\mathcal{F} \pm \nu + 1)]^{\frac{1}{2}} |N\mathcal{F}\nu \pm 1\rangle, \quad (68.26a)$$

$$\hat{F}_o|N\mathcal{F}\nu\rangle = \nu |N\mathcal{F}\nu\rangle. \quad (68.26b)$$

To get the internal energy

$$E(N, \mathcal{F}, \alpha), \quad (68.27)$$

with α indicating the rest of the indices, we need to evaluate the determinant of the $(2\mathcal{F}+1) \times (2\mathcal{F}+1)$ matrix whose elements are (68.24) and equate it to zero. This gives us a numerical equation of degree $4(2\mathcal{F}+1)$ in the variable E^2 and its solution provides us with the values indicated symbolically in (68.27).

We shall discuss the results for $N = 0, 1, 2$ and different values of ω . We start with

$$N = \mathcal{F} = \nu = 0, \quad (68.28)$$

which implies that

$$\langle 000 | \hat{\Pi}_s^2 | 000 \rangle = 1, \quad s = 1, 2, 3, \quad (68.29)$$

and so A, B, C^2 of (68.4) become, respectively,

$$A = 3, \quad B = -3, \quad C^2 = 16, \quad (68.30)$$

and Eq. (68.3) for the energy is given by

$$E^8 - 12E^6 + 30E^4 - 28E^2 + 9 = 0, \quad (68.31)$$

whose four roots for E^2 are $E^2 = 1$, repeated three times, and $E^2 = 9$, which lead to the values $E = \pm 3$ and $E = \pm 1$ as expected from (68.1). In this case of course the value of the energy is independent of ω .

When $N = 1$ we have $\mathcal{F} = 1/2$, $\nu = \pm 1/2$ and if we calculate the matrix elements (68.24) using (68.25,26) we see that the 2×2 matrix is a multiple of the unit matrix, whose coefficient, when equated to 0 gives the fourth degree algebraic equation in E^2 of the form

$$\begin{aligned} E^8 - 4(2\omega + 3)E^6 + [(56/3)\omega^2 + 40\omega + 30]E^4 \\ - [(32/27)\omega^3 + (80/3)\omega^2 + 56\omega + 28]E^2 \\ + [(4/3)\omega^2 - 4\omega - 3]^2 = 0. \end{aligned} \quad (68.32)$$

The roots of this equation will be the energy levels, for the problem and now they do depend on the frequency ω .

We start with ω small compared to 1 which in ordinary units (68.1) means $\hbar\omega \ll mc^2$ and take, for example, $\omega = 0.1$ thus getting an algebraic equation whose roots E^2 are

$$E^2 = 0.9095, 1.0635, 1.2363, 9.5906. \quad (68.33)$$

As we expect these values are close to 1 and 9, that were the values obtained in Eq. (68.31) to which (68.32) reduces when $\omega = 0$. We note though that if we wish only to consider the root corresponding to positive energy close to $E = 3$, then the value of interest to us is $E = 3.096$, which is the positive square root of the largest E^2 appearing above.

When $\omega = 1$, we get an algebraic equation whose roots E^2 are

$$E^2 = 0.4061, 1.4565, 3.7821, 14.3554. \quad (68.34)$$

We now are already well separated from the values 1 and 9 but the roots are still real and positive. On the other hand when, for example, $\omega = 10$, the roots E^2 of Eq. (68.32) take complex values:

68. THE SYSTEM OF THREE RELATIVISTIC

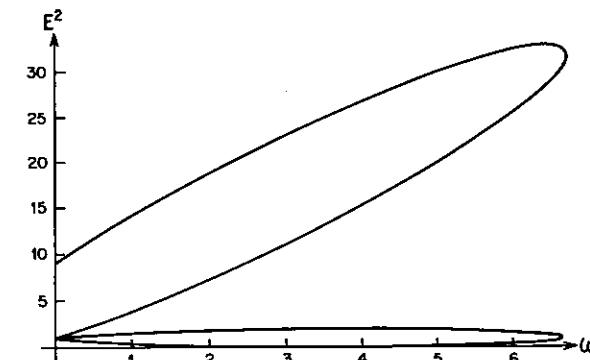


Figure XIII.1. Square of the energy for $N = 1$ given by Eq. (68.32), as function of the frequency ω of the oscillator. For $\omega = 0$ the E^2 are 1 and 9 with the former being triply degenerate. Later they evolve as shown in the figure, but after $\omega = 6.7$ they become complex and are no longer drawn. Note the coincidence of pairs of the levels at the limiting frequency $\omega = 6.7$.

$$E^2 = 0.9659 \pm i1.7083, \quad 45.034 \pm i9.5265. \quad (68.35)$$

This result seems at first sight nonsensical, but we must remember that Dirac, when discussing the exact solution of his equation for a Coulomb potential in its time-like component gets, in our units, the formula [3]

$$E_{nj} = [1 + \gamma^2(s + n)^{-2}]^{-1/2}, \quad (68.36)$$

where $n = 0, 1, 2, 3, \dots$, $s = [(j + \frac{1}{2})^2 - \gamma^2]^{1/2}$, and γ^2 is the fine structure constant which for a nucleus of charge Z is given by $\gamma^2 = (Ze^2/\hbar c) = (Z/137)$. Thus, for example, if $j = 1/2$ and $n = 0$, we have the energy levels

$$E_{01/2} = [1 + \gamma^2(1 - \gamma^2)^{-1}]^{-1/2}, \quad (68.37)$$

and if $Z > 137$, we have that $E_{01/2}$ becomes complex.

Turning to our problem, the fact that after a certain value of ω (which in our case turns out to be $\omega \approx 6.7$, as illustrated in Fig. XIII.1) our energy levels become complex, implies that we can no longer think that the part of positive energies makes sense. Note that at the value of $\omega = 6.7$ indicated in Fig. XIII.1, the level coming from 9 and one of those coming from 1 intersect as do the other two coming from 1.

In fact Pauli and Weisskopf [4], and later others, showed that for very strong interactions, *i.e.*, in our case $\omega > 1$, we can no longer speak of a

fixed number of particles as pairs can be created even if particles obey Bose statistics.

Turning now our attention to the case when $N = 2$ we have, from the argument following Eq. (68.20), that $\mathcal{F} = 1$ or $\mathcal{F} = 0$. In the first case $\nu = 1, 0, -1$ and we have a 3×3 matrix, while in the second there is only a 1×1 matrix. The former, *i.e.*, $\mathcal{F} = 1$ in fact breaks into a 2×2 and 1×1 matrices related respectively to $\nu = 1, -1$ and $\nu = 0$. The 2×2 matrix can be diagonalized in a trivial way using a transformation of the type (61.15), so that finally we get for $\mathcal{F} = 1$ the following algebraic equations:

$$\begin{aligned} E^8 - 4(4\omega + 3)E^6 + (64\omega^2 + 80\omega + 30)E^4 \\ - 4[7 + 28\omega + 32\omega^2 + (256/27)\omega^3]E^2 + (8\omega + 3)^2 = 0, \end{aligned} \quad (68.38a)$$

$$\begin{aligned} E^8 - 4(4\omega + 3)E^6 + [(224/3)\omega^2 + 80\omega + 30]E^4 \\ - 4[7 + 28\omega + (80/3)\omega^2 + (64/27)\omega^3]E^2 \\ + [8\omega + 3 - (16/3)\omega^2]^2 = 0. \end{aligned} \quad (68.38b)$$

Equation (68.38a) corresponds to $\mathcal{F} = 1$ and $\nu = 0$ and to one of the solutions of $\mathcal{F} = 1, \nu \pm 1$, while Eq. (68.38b) corresponds to the other solution of $\mathcal{F} = 1, \nu = \pm 1$. For the case $\mathcal{F} = 0$ and $\nu = 0$ we have the equation

$$\begin{aligned} E^8 - 4(4\omega + 3)E^6 + [(160/3)\omega^2 + 80\omega + 30]E^4 - 4[(448/27)\omega^3 \\ + (112/3)\omega^2 + 28\omega + 7]E^2 + [8\omega + 3 + (16/3)\omega^2]^2 = 0, \end{aligned} \quad (68.39)$$

which happens to have the exact analytic roots

$$E^2 = [1 + (4/3)\omega] \text{ triply degenerate and } E^2 = (9 + 12\omega). \quad (68.40)$$

For $\omega = 0.1$ we get respectively the following roots for E^2 from Eqs. (68.38a), (68.38b) and (68.39):

$$0.9139, \quad 1.1274, \quad 1.3764, \quad 10.1823, \quad (68.41a)$$

$$0.8295, \quad 1.1215, \quad 1.4844, \quad 10.1645, \quad (68.41b)$$

$$1.1333, \quad 1.1333, \quad 1.1333, \quad 10.2. \quad (68.41c)$$

As we should expect all the roots are either close to 1 (triply degenerate) for $\omega = 0$, or close to 9. As we said before it is the root close to $E = 3$, *i.e.*, $E^2 = 9$ that has a physical interest.

For $\omega = 1$ we get respectively the following roots for E^2 from Eqs. (68.38a), (68.38b) and (68.39):

$$0.5558, \quad 2.0328, \quad 5.3338, \quad 20.0776, \quad (68.42a)$$

$$0.1390, \quad 1.6923, \quad 7.1943, \quad 18.9743, \quad (68.42b)$$

$$2.3333, \quad 2.3333, \quad 2.3333, \quad 21.0000. \quad (68.42c)$$

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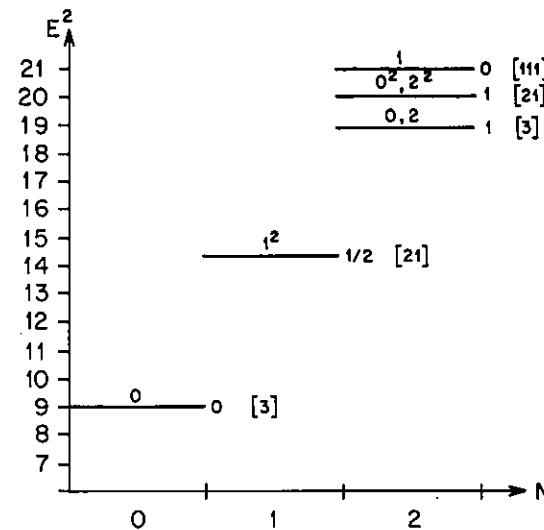


Figure XIII.2. The square of the energy E^2 , as function of the number of quanta N as given by Eqs. (68.31, 32, 38, 39, 40) when $\omega = 1$. The values of \mathcal{F} are given on the right of each level and the possible orbital angular momenta, with their degeneracies, are given above each level. As the function $\phi(E^2, \Pi_s^2)$ is invariant under permutation of the three particles the irreps of $S(3)$ *i.e.* $\{3\}, \{21\}, \{111\}$ characterize the levels as discussed in Table XIII.2, and are also indicated in Fig. XIII.2. In the figure the irreps of $S(3)$ were indicated by square brackets as it was difficult to draw the curly ones.

They are now quite separated from the values of E^2 when $\omega = 0$, *i.e.*, 1 and 9, but the ones that are probably correlated with the latter, are the last ones in each row.

Finally for $\omega = 10$ we get respectively the following roots for E^2 from Eqs. (68.38a), (68.38b) and (68.39):

$$0.1353, \quad 8.8242, \quad 51.8973, \quad 111.143, \quad (68.43a)$$

$$1.0712 \pm i4.9498, \quad 84.9288 \pm i26.348, \quad (68.43b)$$

$$14.333, \quad 14.333, \quad 14.333, \quad 129. \quad (68.43c)$$

At this value of ω all the roots of Eq. (68.38b) are complex, while those of (68.39a) and (68.38) remain real. As the algebraic equations for E^2 have real coefficients, the complex roots are associated with their conjugate, as shown by the \pm signs that appear before the imaginary values in (68.43).

In Fig. XIII.2 we plot the largest real levels for the square of the energy as functions of ω , and will also indicate the possible angular momenta associated with these levels, as will be discussed in the next subsection.

a) The wave function for the relativistic three-body oscillator problem

In (68.23) we denoted our states as linear combinations of $|N\mathcal{F}\nu\rangle$, because we only needed their behavior with respect to the indices $s, t = 1, 2$ to calculate the matrix element of \hat{C}_{st} with respect to them and get the energy eigenvalues. Actually our states depend on the six coordinates \dot{x}_{is} , $i = 1, 2, 3$, $s = 1, 2$, or, equivalently, are polynomials in the six creation operators $\dot{\eta}_{is}$, $i = 1, 2, 3$, $s = 1, 2$, acting on the ground state. Thus the states are associated with the irreducible symmetric representation of a U(6) group characterized by the total number of quanta N , and for which we take the following chain of subgroups:

$$\begin{array}{c} U(6) \supset SU(3) \otimes U(2) \\ \cup \quad \cup \\ L \quad O(3) \quad SU(2) \quad \mathcal{F} \\ \cup \quad \cup \\ M \quad O(2) \quad O(2) \quad \nu, \end{array} \quad (68.44)$$

where either above or to the side we have put the irreps of the groups that characterize the wave function.

Our states can then be denoted by the ket

$$\left| \begin{array}{c} \lambda\mu \\ qLM \\ \nu \end{array} \right\rangle, \quad (68.45)$$

where we used the notation $(\lambda\mu)$ for irreps of SU(3) discussed in Chapter 7, and as indicated there the $(\lambda\mu)$ and (N, \mathcal{F}) are related by

$$N = \lambda + 2\mu, \quad (68.46a)$$

$$\mathcal{F} = (\lambda/2). \quad (68.46b)$$

We add an index q , which replaces the α indicated in Chapter 7, to distinguish between the repeated irreps L of $O(3)$ that are contained in a state with a given irrep $(\lambda\mu)$ of SU(3).

There is also another restriction that we wish to impose on our wave function. As Eq. (68.6) that determines the states is invariant under permutation of its indices $s = 1, 2, 3$, we would like our states to be characterized by the irreps of the permutation group of the three particles, *i.e.*,

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$f \equiv \{3\}, \{2\}, \{111\}$, as well as the corresponding Yamanouchi symbol r as discussed in section 17.

To achieve this last purpose it is convenient, as indicated in (17.10), to introduce the new creation operators through unitary transformation:

$$\begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix} \begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{bmatrix}, \quad (68.47a)$$

which imply that their hermitian conjugates, that are the annihilation operators, satisfy

$$[\xi_1 \xi_2] = [\dot{\xi}_1 \dot{\xi}_2] \frac{1}{\sqrt{2}} \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix}. \quad (68.47b)$$

The matrix of generators \hat{C} in our Jacobi coordinates, and C in the new ones are then given by

$$\hat{C} = \begin{bmatrix} \dot{\eta}_1 \\ \dot{\eta}_2 \end{bmatrix} \cdot [\xi_1 \xi_2], \quad (68.48a)$$

$$C = \begin{bmatrix} \eta_1 \\ \eta_2 \end{bmatrix} \cdot [\dot{\xi}_1 \dot{\xi}_2], \quad (68.48b)$$

and expressing them in their components, and making use of (68.47), we have the relation

$$\begin{bmatrix} \hat{C}_{11} & \hat{C}_{12} \\ \hat{C}_{21} & \hat{C}_{22} \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} i & -i \\ 1 & 1 \end{bmatrix} \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} -i & 1 \\ i & 1 \end{bmatrix}. \quad (68.49)$$

As the matrices appearing on the left and right hand side of (68.49) are the inverse of each other, we see that the Casimir operators of first and second order of the U(2) group are identical:

$$\text{tr}\hat{C} = \text{tr}C, \quad (68.50a)$$

$$\text{tr}\hat{C}^2 = \text{tr}C^2. \quad (68.50b)$$

Furthermore, from (17.8) or (17.10) they are invariant under permutation of the particles.

Thus, in particular, the operator

$$\begin{aligned} \hat{F}^2 &= \frac{1}{2}[\text{tr}C^2 - \frac{1}{2}(\text{tr}C)^2] \\ &= C_{21}C_{12} + \frac{1}{4}[(C_{11} - C_{22})(C_{11} - C_{22} + 2)], \end{aligned} \quad (68.51)$$

will together with \hat{N} characterize the states corresponding to the irrep $(\lambda\mu)$ of our SU(3) group through relations (68.46). Now we turn to Eqs. (17.23, 24, 27) to get the states

$$\phi(n_1 l_1, n_2 l_2, LM; fr), \quad (68.52)$$

where we replaced Λ by L for the total angular momentum, and f is the partition corresponding to the irreps of $S(3)$, i.e., $\{3\}, \{21\}, \{111\}$ while r continues to correspond to the Yamanouchi symbol as discussed in section 17.

Clearly the states (68.52) are characterized by the eigenvalues

$$N = 2n_1 + l_1 + 2n_2 + l_2, \quad |\nu| = |2n_1 + l_1 - 2n_2 - l_2|, \quad L, M, \quad (68.53)$$

but not by the eigenvalue $\mathcal{F}(\mathcal{F}+1)$ of (68.51). Thus what we need is to calculate the matrix elements of \hat{F}^2 with respect to the states ϕ of (68.52) keeping N , $|\nu|$, L , M , f and r fixed, and later diagonalize it. As from (17.23, 24, 27) we see that the states ϕ are a linear combination of at most two kets of the form $|n_1 l_1, n_2 l_2, LM\rangle$ of (10.10), it is sufficient to calculate matrix elements of the form

$$\langle n'_1 l'_1, n'_2 l'_2, LM | C_{st} | n_1 l_1, n_2 l_2, LM \rangle, \quad (68.54)$$

to get that of \hat{F}^2 of (68.51). Those of C_{11} and C_{22} are diagonal and are given respectively by $(2n_1 + l_1)$, $(2n_2 + l_2)$, while those of C_{21} can be calculated by hermitian conjugation from C_{12} , and the latter can be obtained by standard Racah algebra, together with the use of the reduced matrix element (10.35).

Thus we have a straightforward procedure to get the wave functions (68.45) and those of the three-body problem discussed in this section require only the coefficients a_ν in Eq. (68.23), that arise in the process of diagonalizing the matrix in Eq. (68.24).

b) Poincaré invariance of the three-body relativistic equation with oscillator interactions

To express Eq. (68.6) in a Poincaré invariant form we start with definition of the total four momentum for the three particle problem, i.e.,

$$P_\mu = p_{\mu 1} + p_{\mu 2} + p_{\mu 3}, \quad (68.55)$$

where $\mu = 0, 1, 2, 3$ with p_{os} , $s = 1, 2, 3$, being the time-like component while p_{is} , $i = 1, 2, 3$, are the space-like components corresponding to the vector p_s of the previous section.

We shall require also a unit time-like four vector u_μ defined as in (62.53) and which we shall write as

$$u_\mu = P_\mu (-g^{\sigma\tau} P_\sigma P_\tau)^{-\frac{1}{2}}, \quad (68.56)$$

where repeated indices σ, τ are summed over 0, 1, 2, 3 and our contravariant metric tensor is taken as

$$g^{\sigma\tau} = 0 \quad \text{if} \quad \sigma \neq \tau, \quad g^{11} = g^{22} = g^{33} = -g^{00} = 1. \quad (68.57)$$

Clearly in the center of mass frame where $P_i = 0$, $i = 1, 2, 3$, u_μ takes the value

$$(u_\mu) = (1, 0, 0, 0). \quad (68.58)$$

The operators $\dot{\eta}_s$ and $\dot{\xi}_s$, $s = 1, 2$, defined in (68.11) are space-like three-component vectors which could be denoted by $\dot{\eta}_{is}$ or $\dot{\xi}_{is}$, $i = 1, 2, 3$. A time-like component could be added through the definition (68.11) just by putting \dot{p}_{os} or \dot{x}_{os} instead of \dot{p}_{is} or \dot{x}_{is} and thus we would get $\dot{\eta}_{os}$ and $\dot{\xi}_{os}$ which, together with $\dot{\eta}_{is}$ and $\dot{\xi}_{is}$, form the four vectors

$$\dot{\eta}_{\mu s}, \dot{\xi}_{\mu s}; \quad \mu = 0, 1, 2, 3; \quad s = 1, 2. \quad (68.59)$$

We do not want to use these operators directly in the definition of the \dot{C}_{st} of (68.14), but rather utilize their transversal parts defined by

$$\dot{\eta}_{\perp \mu s} \equiv \dot{\eta}_{\mu s} + (g^{\sigma\tau} \dot{\eta}_{\sigma s} u_\tau) u_\mu, \quad (68.60a)$$

$$\dot{\xi}_{\perp \mu s} \equiv \dot{\xi}_{\mu s} + (g^{\sigma\tau} \dot{\xi}_{\sigma s} u_\tau) u_\mu. \quad (68.60b)$$

These transverse operators have the property that in the center of mass frame where $(u_\mu) = (1000)$ we have, because of the metric (68.57), that

$$\dot{\eta}_{\perp os} = 0, \quad \dot{\xi}_{\perp os} = 0, \quad \dot{\eta}_{\perp is} = \dot{\eta}_{is}, \quad \dot{\xi}_{\perp is} = \dot{\xi}_{is}. \quad (68.61)$$

Thus now the generator \dot{C}_{st} , $s, t = 1, 2$, appearing in the definitions (68.13) of $\hat{\Pi}_1^2$, $\hat{\Pi}_2^2$ and $\hat{\Pi}_3^2$ can be expressed in a Lorentz invariant way by

$$\dot{C}_{st} = g^{\sigma\tau} \dot{\eta}_{\perp \sigma s} \dot{\xi}_{\perp \tau t}, \quad (68.62)$$

as in the center of mass frame it takes the form (68.14), i.e., $\dot{C}_{st} = \dot{\eta}_s \cdot \dot{\xi}_t$.

As for the energy E^2 appearing in Eq. (68.6) it can be substituted by the operator

$$E^2 \rightarrow (-g^{\sigma\tau} P_\sigma P_\tau), \quad (68.63)$$

because in the center of mass frame $P_i = 0$, $i = 1, 2, 3$, and from the metric tensor (68.57), we see that the parenthesis in (68.63) reduces to P_o^2 , which is the time-like component of the four momentum vector squared and thus corresponds to the square of the total energy of the system.

With the definitions (68.62) of \dot{C}_{st} and (68.63) of E^2 substituted in Eq. (68.6) we get a Poincaré invariant equation for our problem, as \dot{C}_{st} , given in terms of Jacobi coordinates and momenta, is also invariant under translation in space time, and thus commutes with P_μ .

We have then arrived at a procedure for deriving a Poincaré invariant equation for a three particle system with oscillator interactions which, in the center of mass reference frame, can be solved by a simple group theoretical procedure, which leads eventually to algebraic equations of degree $4(2f+1)$ for E^2 , that can be solved numerically to give the spectrum of the problem.

69 The System of Three Relativistic Spinorial Particles with a Dirac Oscillator Interaction

We shall begin by deriving the Poincaré invariant equation for an n -particle system with Dirac oscillator interactions, by starting from the corresponding problem where we have n -free particles which leads to Eq. (61.31). We first rewrite this equation by expressing it, instead of the linear four momenta of each particle, *i.e.*, $p_{\mu s}$, $\mu = 0, 1, 2, 3$, $s = 1, 2, \dots, n$, by the relative momenta

$$p'_{\mu s} = p_{\mu s} - n^{-1}P_\mu, \quad (69.1)$$

as well as in terms of the total four momentum P_μ of (61.35). In that case Eq. (61.31) takes the form

$$\left[n^{-1} \sum_{s=1}^n \Gamma_s (\gamma_s^\mu P_\mu) + \sum_{s=1}^n \Gamma_s (\gamma_s^\mu p'_{\mu s} + 1) \right] \psi = 0, \quad (69.2)$$

where Γ_s and Γ are defined in (61.30) and the γ_s^μ by (61.28,29), and we assume all the particles of the same mass and use units in which $\hbar = m = c = 1$.

To introduce then a Dirac oscillator interaction we proceed as in Eq. (62.52) by making the replacement

$$p'_{\mu s} \rightarrow p'_{\mu s} - i\omega x'_{\perp \mu s} \Gamma, \quad (69.3)$$

where $x'_{\perp \mu s}$ is the transverse part, of the form (62.50), of the relative four vector coordinate $x'_{\mu s} = x_{\mu s} - X_\mu$ of (62.51). Thus we arrive finally at the equation

$$\left\{ n^{-1} \sum_{s=1}^n \Gamma_s (\gamma_s^\mu P_\mu) + \sum_{s=1}^n [\gamma_s^\mu (p'_{\mu s} - i\omega x'_{\perp \mu s} \Gamma) + 1] \right\} \psi = 0. \quad (69.4)$$

We note that, as in (61.31) and (62.52), we have the unit time like four vector u_μ , $\mu = 0, 1, 2, 3$, appearing in Γ_s and Γ , which is taken as the function (62.53) of the total momentum so that it takes its form $(u_\mu) = (1, 0, 0, 0)$ in the reference frame in which the center of mass is at rest, *i.e.*, when $P_i = 0$, $i = 1, 2, 3$, and $P_o = -P^o = -E$. Going then to this frame of reference, we see by a reasoning entirely similar to the one that carries us from (61.31) to (61.34), that we arrive finally at the equation

$$\sum_{s=1}^n [\alpha_s \cdot (p'_s - i\omega x'_s B) + \beta_s] \psi = E \psi, \quad (69.5)$$

where

$$B = \beta_1 \otimes \beta_2 \otimes \dots \otimes \beta_{n-1} \otimes \beta_n, \quad (69.6)$$

and x'_s and p'_s are the spatial part of the $x'_{\mu s}$ and $p'_{\mu s}$ defined above.

We shall now restrict Eq. (69.5) to the case with $n = 3$, so we can apply it in the next section to a system of three quarks and discuss the mass spectra of non-strange baryons.

As in the case of one particle where in (59.4) we expressed ψ in terms of ψ_τ , $\tau = 1, 2$, the large and the small components, or in the case of two particles when we wrote it in terms of $\psi_{\tau_1 \tau_2}$, $\tau_1, \tau_2 = 1, 2$, so we had four components, in Eq. (69.6) when $n = 3$ we need to express ψ in terms of $\psi_{\tau_1 \tau_2 \tau_3}$, where $\tau_s = 1, 2$, $s = 1, 2, 3$, *i.e.*, we have now eight components.

When dealing with the two-body problem we saw that in Eq. (62.8a,b) we could eliminate the components ψ_{12} and ψ_{21} and get an equation involving only ψ_{11} and ψ_{22} or ϕ_+ and ϕ_- related to the former by (61.15) and satisfying Eq. (62.9).

A similar procedure will serve us to simplify Eq. (69.5) when $n = 3$, so as to be able to calculate the eigenvalues E in the frame of reference where the center of mass is at rest. Let us first denote by Δ the expression

$$\Delta \equiv 3 + \tau_1 + \tau_2 + \tau_3, \quad (69.7)$$

so that $\psi_{\tau_1 \tau_2 \tau_3}$ can be separated into two parts depending on whether Δ is even or odd and which we shall indicate respectively by Ψ_+ and Ψ_- , *i.e.*,

$$\Psi_+ = \begin{bmatrix} \psi_{111} \\ \psi_{122} \\ \psi_{212} \\ \psi_{221} \end{bmatrix}, \quad (69.8a)$$

$$\Psi_- = \begin{bmatrix} \psi_{112} \\ \psi_{121} \\ \psi_{211} \\ \psi_{222} \end{bmatrix}. \quad (69.8b)$$

Equation (66.5) can then be written, by a reasoning similar to the one leading us from (62.4) to (62.8), in the form [5]

$$M\Psi_- = D_+\Psi_+, \quad (69.9a)$$

$$M^\dagger\Psi_+ = D_-\Psi_-, \quad (69.9b)$$

where M^\dagger is the hermitian conjugate of M and

$$M = 2i\sqrt{2\omega} \begin{pmatrix} S_3 \cdot \eta'_3 & S_2 \cdot \eta'_2 & S_1 \cdot \eta'_1 & 0 \\ S_2 \cdot \eta'_2 & S_3 \cdot \eta'_3 & 0 & S_1 \cdot \eta'_1 \\ S_1 \cdot \eta'_1 & 0 & S_3 \cdot \eta'_3 & S_2 \cdot \eta'_2 \\ 0 & S_1 \cdot \eta'_1 & S_2 \cdot \eta'_2 & S_3 \cdot \eta'_3 \end{pmatrix}, \quad (69.10)$$

in which $S_u = (\sigma_u/2)$ and $u = 1, 2, 3$ refer to the index of the three particles while

$$\eta'_u = \eta_u - \frac{1}{3}(\eta_1 + \eta_2 + \eta_3), \quad (69.11a)$$

$$\xi'_u = \eta'^{\dagger}_u, \quad (69.11b)$$

with η_u , $u = 1, 2, 3$, being the usual creation operators associated with the particles. Furthermore D_+ and D_- are constant 4×4 diagonal matrices given by

$$D_+ = \begin{pmatrix} E-3 & & & \\ & E+1 & & \\ & & E+1 & \\ & & & E+1 \end{pmatrix}, \quad (69.12a)$$

$$D_- = \begin{pmatrix} E-1 & & & \\ & E-1 & & \\ & & E-1 & \\ & & & E+3 \end{pmatrix}. \quad (69.12b)$$

Eliminating Ψ_- between the two equations (69.9a,b) we get that Ψ_+ satisfies

$$\mathcal{O}\Psi_+ \equiv [MD_-^{-1}M^\dagger - D_+] \Psi_+ = 0, \quad (69.13)$$

where \mathcal{O} is just a short hand notation for the operator appearing there.

We proceed to find the eigenvalues E and the corresponding eigenfunctions Ψ_+ of (69.13) by first introducing the Jacobi coordinates and momenta by the definitions

$$\dot{x}_1 = (1/\sqrt{2})(x_1 - x_2), \quad \dot{x}_2 = (1/\sqrt{6})(x_1 + x_2 - 2x_3), \quad (69.14)$$

$$\dot{p}_1 = (1/\sqrt{2})(p_1 - p_2), \quad \dot{p}_2 = (1/\sqrt{6})(p_1 + p_2 - 2p_3), \quad (69.15)$$

and in terms of them we introduce the number operator

$$\hat{N} = \frac{1}{2}(\dot{p}_1^2 + \dot{x}_1^2) + \frac{1}{2}(\dot{p}_2^2 + \dot{x}_2^2) - 3, \quad (69.16)$$

as well as the total, orbital and spin angular momenta by

$$\mathbf{J} = \mathbf{L} + \mathbf{S}, \quad (69.17)$$

where

$$\mathbf{L} = (\dot{x}_1 \times \dot{p}_1) + (\dot{x}_2 \times \dot{p}_2), \quad (69.18a)$$

$$\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3. \quad (69.18b)$$

Clearly both \hat{N} and \mathbf{J} , as well as J^2 and J_3 , are integrals of motion of our problem as they commute with \mathcal{O} , and the eigenstates of the latter are linear combinations of

$$|n_1\ell_1, n_2\ell_2(L); \frac{1}{2}\frac{1}{2}(T)\frac{1}{2}(S); JM\rangle = \left[\left[(\dot{x}_1|n_1\ell_1) \times (\dot{x}_2|n_2\ell_2) \right]_L \times \left[\left[(1|\frac{1}{2}) \times (2|\frac{1}{2}) \right]_T \times (3|\frac{1}{2}) \right]_S \right]_{JM}, \quad (69.19)$$

where $2n_1 + \ell_1 + 2n_2 + \ell_2 = N$, with N being the eigenvalue of \hat{N} , and the square brackets indicate angular momentum coupling to the values indicated by their indices.

If the values N and J are fixed we have just a finite number of states of the type (69.19) and thus the matrix of the operator \mathcal{O} of (69.13) with respect to these states will be finite. Its determinant equated to 0 will give an algebraic equation in the parameter E , and its solution provides the eigenvalues of the energy for the relativistic three-body problem with a Dirac oscillator interaction. As this energy E is given in the frame of reference where the center of mass is at rest, we can interpret it, in our units $\hbar = m = c = 1$, as the mass spectrum of the composite particle, formed from three more elementary ones. The case of particular interest is the one in which these three particles are quarks, and thus the objective of the following subsection is to discuss their symmetries.

a) Symmetries of the systems of three quarks

It is well known that the wave functions [5] of a system of three quarks have an orbital, spin, flavor and color parts. As all baryons are colorless the color part must be antisymmetric under the interchange of the quarks. As the latter are fermions the total wave function must also be antisymmetric under the interchange of the quarks. Thus the orbital, spin and flavor parts of the wave functions must be symmetric under the permutation group $S(3)$ associated with the three quarks. We are only going to discuss the non strange baryons that are formed either by up(u) or down(d) quarks that have the same mass, and thus all quarks can be taken, in our units, as of mass 1.

The orbital part of our wave functions can be written in terms of Jacobi vectors for the coordinates \dot{x}_1, \dot{x}_2 of (69.14) as

$$(\dot{x}_1, \dot{x}_2 | n_1 l_1, n_2 l_2, LM), \quad (69.20)$$

as in (10.10) and (1.2). Furthermore in Eq. (17.32) we show what linear combinations of these states, with fixed N and L , are required to give definite irreps $f = \{3\}, \{21\}, \{111\}$ of $S(3)$ group, as well as their corresponding Yamanouchi's symbols r .

In our calculations for the baryon mass spectra, that will be presented later, we will only be interested in orbital states up to $N = 2$. Thus rather than repeat the discussion of section 17, we first indicate in Table XIII.1 a short hand notation for the 10 states of the form (69.20) that go up to $N = 2$ quanta, and then in Table XIII.2 we give the linear combination of them that correspond to definite irrep $f = \{3\}, \{21\}, \{111\}$ of $S(3)$ and which we denote by $|NLfr\rangle$. Furthermore as in the case of $\{21\}$ there are two possibilities for the Yamanouchi symbols $r = (211)$ and $r = (121)$, as indicated in (17.23) and (17.24), we shall use for them respectively the short hand notation $r = 1$ and $r = 2$. For $\{3\}, \{111\}$, as there is only one Yamanouchi symbol it will not be given.

Turning now our attention to the spin of three particles we notice immediately that when $s = (3/2)$ it belongs to $f = \{3\}$ as can be seen immediately if we consider the projection $\frac{3}{2}$ itself, which is the product of three states of projection $\frac{1}{2}$ for the spin of each particle. For the spin $s = (1/2)$ the irrep of $S(3)$ [6] is $\{21\}$ with $r = 1$ or 2 depending on whether the in the spin part of Eq. (69.19) is $T = 1$ or 0.

When coupling the orbital and spin states, each with definite permutational symmetry, to a total J , we can get a final orbital spin state corresponding to an irrep of $S(3)$, by using well known projection techniques [6]. We shall denote these states by the ket

$$|NLf'; S; JM; fr\rangle, \quad (69.21)$$

Table XIII.1. Compact notation $|L_\beta\rangle$ for orbital states of the three-quark system.

$$\begin{aligned} |00, 00, 0\rangle &= |0\rangle, & |01, 00, 1\rangle &= |1_1\rangle, & |00, 01, 1\rangle &= |1_2\rangle, \\ |02, 00, 2\rangle &= |2_1\rangle, & |00, 02, 2\rangle &= |2_2\rangle, & |01, 01, 2\rangle &= |2_3\rangle, \\ |10, 00, 0\rangle &= |0_1\rangle, & |00, 10, 0\rangle &= |0_2\rangle, & |01, 01, 0\rangle &= |0_3\rangle, \\ |01, 01, 1\rangle &= |1\rangle. \end{aligned}$$

Table XIII.2. Orbital states of the three-quark system adapted to the permutational symmetry $S(3)$ as functions of $|L_\beta\rangle$. The irrep of $S(3)$ is indicated by f and the Yamanouchi symbol by r .

Symmetry adapted orbital states $ NLfr\rangle$	Explicit expression of the states in terms of the $ L_\beta\rangle$ in Table XIII.1
$ 00\{3\}\rangle$	$ 0\rangle$
$ 11\{21\}1\rangle$	$ 1_2\rangle$
$ 11\{21\}2\rangle$	$ 1_1\rangle$
$ 22\{3\}\rangle$	$(1/\sqrt{2})[2_2\rangle + 2_1\rangle]$
$ 22\{21\}1\rangle$	$(1/\sqrt{2})[2_2\rangle - 2_1\rangle]$
$ 22\{21\}2\rangle$	$ 2_3\rangle$
$ 20\{3\}\rangle$	$(1/\sqrt{2})[0_1\rangle + 0_2\rangle]$
$ 20\{21\}1\rangle$	$(1/\sqrt{2})[0_2\rangle - 0_1\rangle]$
$ 20\{21\}2\rangle$	$- 0_3\rangle$
$ 21\{111\}\rangle$	$ 1\rangle$

and in Table XIII.3 we give them, up to $N = 2$, in terms of the kets (69.19), but using the compact notation of Table XIII.1.

Finally we have to mention the states with flavor [5], which belong to the irrep of a $U(3)$ group, which turn out to be [7] exactly the same than those of the permutational group $S(3)$. Thus we can denote these states by

$$|fr, Irs\rangle, \quad (69.22)$$

where I is the irrep of $SU(2)$ subgroup of $U(3)$ that corresponds to the isospin and r its projection while s is the strangeness. As we will only consider states with strangeness $s = 0$, then, as in the case of ordinary spin, we have that when $f = \{3\}$ and $I = (3/2)$, $f = \{21\}$ and $I = (1/2)$, and we can suppress in (70.22) all indices except f and r and write the flavor ket as

Table XIII.3a. Orbital-spin states for the three-quark system adapted to the permutational symmetry $S(3)$. In the ket N stands for a number of quanta, L for the orbital angular momentum, f' for the irrep of $S(3)$ for the orbital part, S for the total spin and T for the spin of the first two particles, J for the total angular momentum, while f is the irrep of $S(3)$ for the whole state and r the Yamanouchi symbol given explicitly only for $f = \{21\}$ in the contracted notation indicated in the text. The orbital states are given in the shorthand notation of Table XIII.1. The round kets on the right-hand side of the table are a shorthand notation for the kets in Eq. (69.19).

N	J	f	r	$ NLf', S, J, fr\rangle = L_\beta, TS, J\rangle$
0	$\frac{3}{2}$	{3}		$ 00\{3\}, \frac{3}{2}, \frac{3}{2}\{3\}\rangle = 0, 1\frac{3}{2}, \frac{3}{2}\rangle$
0	$\frac{1}{2}$	{21}	1	$ 00\{3\}, \frac{1}{2}, \frac{1}{2}\{21\}1\rangle = 0, 1\frac{1}{2}, \frac{1}{2}\rangle$
0	$\frac{1}{2}$	{21}	2	$ 00\{3\}, \frac{1}{2}, \frac{1}{2}\{21\}2\rangle = 0, 0\frac{1}{2}, \frac{1}{2}\rangle$
1	$\frac{5}{2}$	{21}	1	$ 11\{21\}, \frac{3}{2}, \frac{3}{2}\{21\}1\rangle = 1_2, 1\frac{3}{2}, \frac{3}{2}\rangle$
1	$\frac{5}{2}$	{21}	2	$ 11\{21\}, \frac{3}{2}, \frac{3}{2}\{21\}2\rangle = 1_1, 1\frac{3}{2}, \frac{3}{2}\rangle$
1	$\frac{3}{2}$	{3}		$ 11\{21\}, \frac{1}{2}, \frac{3}{2}\{3\}\rangle = \frac{1}{\sqrt{2}}(1_2, 1\frac{1}{2}, \frac{1}{2}\rangle + 1_1, 0\frac{1}{2}, \frac{3}{2}\rangle)$
1	$\frac{3}{2}$	{21}	1	$ 11\{21\}, \frac{3}{2}, \frac{3}{2}\{21\}1\rangle = 1_2, 1\frac{3}{2}, \frac{3}{2}\rangle$
1	$\frac{3}{2}$	{21}	1	$ 11\{21\}, \frac{1}{2}, \frac{3}{2}\{21\}1\rangle = \frac{1}{\sqrt{2}}(1_2, 1\frac{1}{2}, \frac{3}{2}\rangle - 1_1, 0\frac{1}{2}, \frac{3}{2}\rangle)$
1	$\frac{3}{2}$	{21}	2	$ 11\{21\}, \frac{3}{2}, \frac{3}{2}\{21\}2\rangle = 1_1, 1\frac{3}{2}, \frac{3}{2}\rangle$
1	$\frac{3}{2}$	{21}	2	$ 11\{21\}, \frac{1}{2}, \frac{3}{2}\{21\}2\rangle = \frac{1}{\sqrt{2}}(1_2, 0\frac{1}{2}, \frac{3}{2}\rangle + 1_1, 1\frac{1}{2}, \frac{3}{2}\rangle)$
1	$\frac{3}{2}$	{111}		$ 11\{21\}, \frac{1}{2}, \frac{3}{2}\{111\}\rangle = \frac{1}{\sqrt{2}}(1_2, 0\frac{1}{2}, \frac{3}{2}\rangle - 1_1, 1\frac{1}{2}, \frac{3}{2}\rangle)$
1	$\frac{1}{2}$	{3}		$ 11\{21\}, \frac{1}{2}, \frac{1}{2}\{3\}\rangle = \frac{1}{\sqrt{2}}(1_2, 1\frac{1}{2}, \frac{1}{2}\rangle + 1_1, 0\frac{1}{2}, \frac{1}{2}\rangle)$
1	$\frac{1}{2}$	{21}	1	$ 11\{21\}, \frac{3}{2}, \frac{1}{2}\{21\}1\rangle = 1_2, 1\frac{3}{2}, \frac{1}{2}\rangle$
1	$\frac{1}{2}$	{21}	1	$ 11\{21\}, \frac{1}{2}, \frac{1}{2}\{21\}1\rangle = \frac{1}{\sqrt{2}}(1_2, 1\frac{1}{2}, \frac{1}{2}\rangle - 1_1, 0\frac{1}{2}, \frac{1}{2}\rangle)$
1	$\frac{1}{2}$	{21}	2	$ 11\{21\}, \frac{3}{2}, \frac{1}{2}\{21\}2\rangle = 1_1, 1\frac{3}{2}, \frac{1}{2}\rangle$
1	$\frac{1}{2}$	{21}	2	$ 11\{21\}, \frac{1}{2}, \frac{1}{2}\{21\}2\rangle = -\frac{1}{\sqrt{2}}(1_2, 0\frac{1}{2}, \frac{1}{2}\rangle + 1_1, 1\frac{1}{2}, \frac{1}{2}\rangle)$
1	$\frac{1}{2}$	{111}		$ 11\{21\}, \frac{1}{2}, \frac{1}{2}\{111\}\rangle = \frac{1}{\sqrt{2}}(1_2, 0\frac{1}{2}, \frac{1}{2}\rangle - 1_1, 1\frac{1}{2}, \frac{1}{2}\rangle)$
2	$\frac{7}{2}$	{3}		$ 22\{3\}, \frac{3}{2}, \frac{7}{2}\{3\}\rangle = \frac{1}{\sqrt{2}}(2_2, 1\frac{3}{2}, \frac{7}{2}\rangle + 2_1, 1\frac{3}{2}, \frac{7}{2}\rangle)$
2	$\frac{7}{2}$	{21}	1	$ 22\{21\}, \frac{3}{2}, \frac{7}{2}\{21\}1\rangle = \frac{1}{\sqrt{2}}(2_2, 1\frac{3}{2}, \frac{7}{2}\rangle - 2_1, 1\frac{3}{2}, \frac{7}{2}\rangle)$
2	$\frac{7}{2}$	{21}	2	$ 22\{21\}, \frac{3}{2}, \frac{7}{2}\{21\}2\rangle = - 2_3, 1\frac{3}{2}, \frac{7}{2}\rangle$
2	$\frac{5}{2}$	{3}		$ 22\{3\}, \frac{3}{2}, \frac{5}{2}\{3\}\rangle = \frac{1}{\sqrt{2}}(2_2, 1\frac{3}{2}, \frac{5}{2}\rangle + 2_1, 1\frac{3}{2}, \frac{5}{2}\rangle)$
2	$\frac{5}{2}$	{3}		$ 22\{3\}, \frac{1}{2}, \frac{5}{2}\{3\}\rangle = \frac{1}{2}(2_2, 1\frac{1}{2}, \frac{5}{2}\rangle - 2_1, 1\frac{1}{2}, \frac{5}{2}\rangle) - \frac{1}{\sqrt{2}} 2_3, 0\frac{1}{2}, \frac{5}{2}\rangle$
2	$\frac{5}{2}$	{21}	1	$ 22\{21\}, \frac{3}{2}, \frac{5}{2}\{21\}1\rangle = \frac{1}{\sqrt{2}}(2_2, 1\frac{3}{2}, \frac{5}{2}\rangle - 2_1, 1\frac{3}{2}, \frac{5}{2}\rangle)$
2	$\frac{5}{2}$	{21}	1	$ 22\{3\}, \frac{1}{2}, \frac{5}{2}\{21\}1\rangle = \frac{1}{\sqrt{2}}(2_2, 1\frac{1}{2}, \frac{5}{2}\rangle + 2_1, 1\frac{1}{2}, \frac{5}{2}\rangle)$

The Harmonic Oscillator in Modern Physics

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About the authors

Marcos Moshinsky obtained his B.Sc. from the Universidad Nacional Autónoma de México (U.N.A.M.) and his M.A. and Ph.D. from Princeton University. He has received many national and international prizes, and is a member of several scientific academies. Currently he is a professor of physics at U.N.A.M.

Yuri F. Smirnov studied at the Moscow State University, where he received his doctorate in 1972. He received the K.D. Sinelnikov Prize from the Ukrainian Academy of Sciences. Currently, he is a senior researcher at the Instituto de Física at U.N.A.M.

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