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A GENERAL TWO-BODY MATRIX ELEMENT FOR A GAUSSIAN INTERACTION USING CYLINDRICAL HARMONIC OSCILLATOR FUNCTIONS

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Abstract: The two-body matrix element for a Gaussian force is obtained in closed form using cylindrical harmonic oscillator wave functions. The result is completely general allowing all possible cylindrical states and allowing different oscillator constants for each state. These include matrix elements which cannot be determined by the usual methods of separation into relative and centre-of-mass coordinates.

1. Introduction

In recent years there have been a number of calculations [1]) of a limited Hartree-Fock type in order to investigate various dynamical features of nuclei. In most cases the interactions between only the "active" (non-closed shell nucleons) have been considered, with the closed shells being treated as an inert core. However, some recent investigations [2]) on ground state deformations and the properties of excited states formed by excitation of two or more particles out of the closed shells, e.g. the first excited 0^+ state of ^{16}O, have indicated the desirability of considering all interactions between particles without any reference to an inert core. Thus, it is convenient to deal with the translationally invariant Hamiltonian.

$$H = \sum_{i=1}^{A} T_i - T_{\text{c.m.}} + \sum_{i<j=1}^{A} V(r_{ij}), \tag{1.1}$$

where T_i is the particle kinetic energy, $T_{\text{c.m.}}$ the centre-of-mass kinetic energy and $V(r_{ij})$ some appropriate two-particle interaction including various exchange terms. The potential energy is summed over all two-particle interactions.

The main problem is to investigate this Hamiltonian for a large variety of different situations, i.e. different deformations, different nuclear sizes and possibly even different oscillator constants for different nuclear orbitals. In evaluating the Hamiltonian under these general conditions it is of course the evaluation of the two-body interaction matrix elements which causes difficulty. If a Slater determinant representation is used and the orbital oscillator constants are different, then the standard techniques

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of Moshinsky transformations [3]) and Talmi integrals [4]) are no longer valid and some sort of direct evaluation of the spatial matrix elements is needed. Since the number of different matrix elements required by (1.1) can be fairly large, and since equilibrium investigations involving different nuclear sizes and deformations require many repeated evaluations of the matrix elements, time considerations require a rapid and general method for evaluating the desired matrix elements.

Rapidity and convenience imposes the following restrictions on the representation and interaction used. The single-particle wave functions are solutions of a cylindrically symmetric harmonic oscillator with different oscillator constants for the different orbitals. If desired, matrix elements in a spherical representation could be obtained by an appropriate unitary transformation. The radial part of the two-particle interaction is of Gaussian form. This latter restriction is not as severe as might appear since a combination of Gaussians can be used to approximate more realistic interactions. In particular a very successful force, in the spirit of the Scott-Moszkowski separation method [5]), has been used [6]) which is a simple combination of an attractive and a repulsive Gaussian. This force fits the low-energy scattering data, gives good binding energies and sizes for closed shell nuclei in equilibrium calculations and gives a rather good fit to the spectra of the 1p shell nuclei. With the above restrictions it is possible to integrate the matrix elements directly for the most general case and to obtain a result which is amenable to rapid computer computations.

In solving the problem in cylindrical symmetry it is necessary to determine one part of the matrix element (the z-component) in one dimension of a Cartesian basis. Consequently, the following results allow the problem to be studied in a completely Cartesian basis if an asymmetric solution exists as was found in ^{24}Mg in a recent calculation [7]). However, the cylindrically symmetric functions have the advantage of conserving the z-component of angular momentum and thus reducing the number of non-zero matrix elements which must be evaluated.

2. Single-Particle Representation

The wave equation for the three-dimensional harmonic oscillator, in cylindrical coordinates is

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\Psi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\Psi}{\partial\varphi^2}+\frac{\partial^2\Psi}{\partial z^2}+(\lambda-\alpha^2\rho^2-a^2z^2)\Psi = 0, \tag{2.1}$$

where

$$\lambda = \frac{2m}{\hbar^2}E, \qquad \alpha = \frac{m}{\hbar}\omega, \qquad a = \frac{m}{\hbar}\omega_z,$$

E being the energy eigenvalue and ω and ω_z the oscillator frequencies.

Separation of variables leads to the three equations

$$\frac{\mathrm{d}^2Z}{\mathrm{d}z^2}+(\lambda_z-a^2z^2)Z = 0, \tag{2.2}$$

$$\frac{d^2\Phi}{d\varphi^2}+m^2\Phi = 0, \tag{2.3}$$

$$\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{dP}{d\rho}\right)+\left(\lambda'-\alpha^2\rho^2-\frac{m^2}{\rho^2}\right)P = 0, \tag{2.4}$$

where

$$\lambda' = \lambda-\lambda_z.$$

The normalized solutions for the first two equations are well known:

$$Z_{n_z}(z) = \left(\frac{a^{\frac{1}{2}}}{\pi^{\frac{1}{2}}2^n n_z!}\right)^{\frac{1}{2}} H_{n_z}(\sqrt{a}z)e^{-\frac{1}{2}az^2}, \tag{2.5}$$

where $H_{n_z}(\sqrt{a}z)$ is the appropriate Hermite polynomial and n_z can be any positive integer including zero, and

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi}, \tag{2.6}$$

where m can have any integer value.

If the substitution into (2.4) of

$$P(\rho) = (\sqrt{\alpha}\rho)^{|m|}e^{-\frac{1}{2}\alpha\rho^2}F(\rho) \tag{2.7}$$

is made, then $F(\rho)$ must satisfy the equation for the Laguerre polynomial, and the normalized solution for $P(\rho)$ is

$$P_{n,m}(\rho) = \left(\frac{2\alpha n!}{(n+|m|)!}\right)^{\frac{1}{2}}(\sqrt{\alpha}\rho)^{|m|}L_n^{|m|}(\alpha\rho^2)e^{-\frac{1}{2}\alpha\rho^2}, \tag{2.8}$$

where $n = \frac{1}{2}(\frac{1}{2}\lambda'/\alpha-|m|-1)$ can be any positive integer including zero, and where

$$L_p^k(\alpha\rho) = \sum_{s=0}^{p}\mathscr{L}_{ps}^k(\alpha)\rho^s. \tag{2.9}$$

The expansion coefficient has the value

$$\mathscr{L}_{ps}^k(\alpha) = \frac{(p+k)!(-\alpha)^s}{(p-s)!(k+s)!s!}. \tag{2.10}$$

It should be noted that alternative definitions exist for the Laguerre polynomial which would lead to different normalization constants.

The single particle representation is then of the form

$$\psi_{n,m,n_z}(\sqrt{\alpha}\rho,\varphi,\sqrt{a}z) = P_{n,m}(\sqrt{\alpha}\rho)\Phi_m(\varphi)Z_{n_z}(\sqrt{a}z). \tag{2.11}$$

The harmonic oscillator energy associated with this function is

$$E_{n,m,n_z} = (2n+|m|+1)\hbar\omega+(n_z+\tfrac{1}{2})\hbar\omega_z. \tag{2.12}$$

The general matrix element that must be solved is

$$\langle\psi_{n_1,m_1,n_{z_1}}(\sqrt{\alpha}\rho_1, \varphi_1, \sqrt{a}z_1), \psi_{n_2,m_2,n_{z_2}}(\sqrt{\beta}\rho_2, \varphi_2, \sqrt{b}z_2)| \mathrm{e}^{-\frac{1}{2}k((\rho_1-\rho_2)^2+(z_1-z_2)^2)}$$
$$\times |\psi_{n_3,m_3,n_{z_3}}(\sqrt{\gamma}\rho_1, \varphi_1, \sqrt{c}z_1)\psi_{n_4,m_4,n_{z_4}}(\sqrt{\delta}\rho_2, \varphi_2, \sqrt{d}z_2)\rangle$$
$$= M(n_1 m_1 \alpha, n_2 m_2 \beta, n_3 m_3 \gamma, n_4 m_4 \delta; k) I(n_{z_1}a, n_{z_2}b, n_{z_3}c, n_{z_4}d; k), \tag{2.13}$$

M is just the radial and angular part of the matrix element which can be separated from I, the z-part of the matrix element.

3. The Radial and Angular Matrix Element

For convenience we ignore the normalization constants and define the unnormalized radial and angular matrix element as

$$\mathscr{M}(n_1 m_1 \alpha, n_2 m_2 \beta, n_3 m_3 \gamma, n_4 m_4 \delta; k)$$
$$= \iiiint (\sqrt{\alpha}\rho_1)^{|m_1|} L_{n_1}^{|m_1|}(\alpha\rho_1^2)\mathrm{e}^{-\frac{1}{2}\alpha\rho_1^2}\mathrm{e}^{-im_1\varphi_1}(\sqrt{\beta}\rho_2)^{|m_2|}L_{n_2}^{|m_2|}(\beta\rho_2^2)\mathrm{e}^{-\frac{1}{2}\beta\rho_2^2}\mathrm{e}^{-im_2\varphi_2}$$
$$\times \mathrm{e}^{-\frac{1}{2}k(\rho_1^2+\rho_2^2-2\rho_1\rho_2\cos\varphi_{12})}(\sqrt{\gamma}\rho_1)^{|m_3|}L_{n_3}^{|m_3|}(\gamma\rho_1^2)\mathrm{e}^{im_3\varphi_1}\mathrm{e}^{-\frac{1}{2}\gamma\rho_1^2}$$
$$\times (\sqrt{\delta}\rho_2)^{|m_4|}L_{n_4}^{|m_4|}(\delta\rho_2^2)\mathrm{e}^{-\frac{1}{2}\delta\rho_2^2}\mathrm{e}^{im_4\varphi_2}\rho_1\rho_2\mathrm{d}\rho_1\mathrm{d}\rho_2\mathrm{d}\varphi_1\mathrm{d}\varphi_2. \tag{3.1}$$

The angular variables can be chosen as φ_2 and $\chi = \varphi_{12} = \varphi_1 - \varphi_2$. The integration over φ_2 will just give the factor $2\pi\delta_{m_1+m_2-m_3-m_4,0}$, i.e. the selection rule which conserves the z-component of the angular momentum. The other angular integration, which is performed first, gives [8])

$$\int_0^{2\pi} \mathrm{e}^{i(m_3-m_1)\chi}\mathrm{e}^{k\rho_1\rho_2\cos\chi}\mathrm{d}\chi = 2\pi\mathrm{e}^{\frac{1}{2}i(m_3-m_1)\pi}J_{(m_3-m_1)}(-ik\rho_1\rho_2), \tag{3.2}$$

where $J_n(z)$ is the usual Bessel function.

If we define

$$\rho_1' = \sqrt{\lambda}\rho_1, \qquad \lambda = 2(\alpha+\gamma+k)$$

and if we expand all the Laguerre polynomials according to (2.9) the matrix element becomes

$$\mathscr{M} = 4\pi^2\mathrm{e}^{\frac{1}{2}i(m_3-m_1)\pi}\alpha^{\frac{1}{2}|m_1|}\beta^{\frac{1}{2}|m_2|}\gamma^{\frac{1}{2}|m_3|}\delta^{\frac{1}{2}|m_4|}\lambda^{-\frac{1}{2}(|m_1|+|m_3|+2)}$$
$$\times \sum_{r=0}^{n_1}\sum_{s=0}^{n_2}\sum_{t=0}^{n_3}\sum_{u=0}^{n_4}\left[\int_0^\infty\int_0^\infty \rho_1'^{(|m_1|+|m_3|+2r+2t)}\mathrm{e}^{-\frac{1}{2}\rho_1'^2}J_{(m_3-m_1)}\left(-\frac{ik}{\sqrt{\lambda}}\rho_1'\rho_2\right)\rho_1'\mathrm{d}\rho_1'\right.$$
$$\left.\times \rho_2^{|m_2|+|m_4|+2s+2u}\mathrm{e}^{-\frac{1}{2}(\beta+\delta+k)\rho_2^2}\rho_2\mathrm{d}\rho_2\right] \mathscr{L}_{n_1r}^{|m_1|}(\alpha/\lambda)\mathscr{L}_{n_2s}^{|m_2|}(\beta)\mathscr{L}_{n_3t}^{|m_3|}(\gamma/\lambda)\mathscr{L}_{n_4u}^{|m_4|}(\delta). \tag{3.3}$$

The integral over ρ_1 can be integrated by use of the relation

$$\int_0^\infty x^{2n+p+1}e^{-\frac{1}{4}x^2}J_p(xy)\mathrm{d}x = 2^{2n+p+1}n!y^p e^{-y^2}L_n^p(y^2). \tag{3.4}$$

The relation (3.4) is valid when p and n are integers and follows from the general integral form of the Laguerre polynomial [9]) which is valid for any complex value of y and thus can be used in (3.3) where y is a pure imaginary number. Eq. (3.4) can also be used for negative integer order by use of the relation

$$J_{-p}(x) = (-1)^p J_p(x). \tag{3.5}$$

By use of these relations the unnormalized radial and angular matrix element becomes

$$\begin{aligned}\mathscr{M} &= 2^{|m_1|+|m_3|+2}\pi^2\alpha^{\frac{1}{2}|m_1|}\beta^{\frac{1}{2}|m_2|}\gamma^{\frac{1}{2}|m_3|}\delta^{\frac{1}{2}|m_4|}k^{|m_3-m_1|}\\ &\quad\times\lambda^{\frac{1}{2}(|m_2|+|m_4|-|m_1|-|m_3|)}\kappa^{-(|m_3-m_1|+|m_2|+|m_4|+2)}\\ &\quad\times\sum_{r=0}^{n_1}\sum_{s=0}^{n_2}\sum_{t=0}^{n_3}\sum_{u=0}^{n_4}\sum_{v=0}^{n} n!(\tfrac{1}{2}(|m_3-m_1|+|m_2|+|m_4|)+s+u+v)!\\ &\quad\times\mathscr{L}_{n_1r}^{|m_1|}(4\alpha/\lambda)\mathscr{L}_{n_2s}^{|m_2|}(\beta\lambda/\kappa^2)\mathscr{L}_{n_3t}^{|m_3|}(4\gamma/\lambda)\mathscr{L}_{n_4u}^{|m_4|}(\delta\lambda/\kappa^2)\mathscr{L}_{nv}^{|m_3-m_1|}(-k^2/\kappa^2),\end{aligned} \tag{3.6}$$

where

$$\kappa^2 = (\beta+\delta)(\alpha+\gamma)+k(\alpha+\beta+\delta+\gamma),$$
$$2n = |m_1|+|m_3|-|m_3-m_1|+2r+2t.$$

Although five sums are involved in (3.6), the number of terms involved in any given sum is quite small and the matrix element can be evaluated quite easily by machine computation. It should be noted that the extra generality of assuming all possible oscillator constants only adds one summation to (3.6).

4. The Cartesian Matrix Element

The unnormalized Cartesian matrix element

$$\begin{aligned}\mathscr{Q}(n_1a, n_2b, n_3c, n_4d; k) &= \iint H_{n_1}(\sqrt{a}z_1)e^{-\frac{1}{2}az_1^2}H_{n_2}(\sqrt{b}z_2)e^{-\frac{1}{2}bz_2^2}\\ &\quad\times e^{-\frac{1}{2}k(z_1-z_2)^2}H_{n_3}(\sqrt{c}z_1)e^{-\frac{1}{2}cz_1^2}H_{n_4}(\sqrt{d}z_2)e^{-\frac{1}{2}dz_2^2}\mathrm{d}z_1\mathrm{d}z_2\end{aligned} \tag{4.1}$$

can be evaluated by use of the following relations involving Hermite polynomials. First [10]),

$$H_m(\alpha\chi) = \sum_{r=0}^{[m]} h_{mr}(\alpha/\beta)H_{m-2r}(\beta\chi), \tag{4.2}$$

where $[m] = \frac{1}{2}m$ if m is even and $[m] = \frac{1}{2}(m-1)$ if m is odd, and where the expansion coefficient

$$h_{mr}(y) = \frac{m!y^{m-2r}(y^2-1)^r}{r!(m-2r)!}\,; \tag{4.3}$$

second [11]),

$$\int_{-\infty}^{\infty} e^{-(x-y)^2} H_m(\alpha x) H_n(\alpha x) dx$$
$$= \sqrt{\pi} \sum_{k=0}^{\min(m,n)} 2^k k! \binom{m}{k}\binom{n}{k} (1-\alpha^2)^{\frac{1}{2}(m+n-2k)} H_{m+n-2k}\left(\frac{\alpha y}{(1-\alpha^2)^{\frac{1}{2}}}\right), \tag{4.4}$$

where $\binom{m}{k}$ is the binomial coefficient and the upper summation limit is the smallest of either m or n; and finally [12]),

$$\int_{-\infty}^{\infty} e^{-y^2} H_k(y) H_m(y) H_n(y) dy = \frac{\sqrt{\pi}k!m!n!2^s}{(s-k)!(s-m)!(s-n)!}, \tag{4.5}$$

if $2s = k+m+n$ is even otherwise the integral vanishes. The integral also vanishes if any of the terms in the denominator become negative integers, The unnormalized matrix element becomes

$$\mathcal{Q} = 2\pi\kappa^{-1} \sum_{r=0}^{[n_3]} \sum_{s=0}^{\min(n_1, n_3-2r)} \sum_{t=0}^{[n_1+n_3-2r-2s]} \sum_{u=0}^{[n_2]} \sum_{v=0}^{[n_4]} 2^{s+n} s! \binom{n_1}{s}\binom{n_3-2r}{s}$$
$$\times \frac{(n_1+n_3-2r-2s-2t)!(n_2-2u)!(n_4-2v)!}{(n-n_1-n_3+2r+2s+2t)!(n-n_2+2u)!(n-n_4+2v)!} \left(\frac{c-a+k}{a+c+k}\right)^{\frac{1}{2}(n_1+n_3-2r-2s)}$$
$$\times h_{n_3r}\left(\left(\frac{c}{a}\right)^{\frac{1}{2}}\right) h_{(n_1+n_3-2r-2s)t}\left(\left(\frac{ak^2}{(c-a+k)\kappa^2}\right)^{\frac{1}{2}}\right) h_{n_2u}\left(\left(\frac{4b\lambda}{\kappa^2}\right)^{\frac{1}{2}}\right) h_{n_4v}\left(\left(\frac{4d\lambda}{\kappa^2}\right)^{\frac{1}{2}}\right), \tag{4.6}$$

where

$$\lambda = \tfrac{1}{2}(a+c+k),\ 2n = n_1+n_2+n_3+n_4-2r-2s-2t-2u-2v,$$
$$\kappa^2 = (a+c)(b+d)+k(a+b+c+d).$$

Since $2n$ must be an even number for (4.6) to be non-vanishing, we see that n_1+n_2+ $+n_3+n_4$ must be even to obtain a non-vanishing matrix element.

The proper normalized two-body matrix element can be obtained by multiplying (3.5) and (4.6) with the appropriate normalization constants as given by (2.5) and (2.8) and then multiplying the two normalized matrix elements together.

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