

RESONATING GROUP CALCULATIONS IN LIGHT NUCLEAR SYSTEMS

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1. INTRODUCTION

Already in the early times of nuclear physics Wheeler /WH 37/ invented the Resonating Group Method (RGM). In close analogy to the molecular binding he studied nuclear few body system. His idea becomes most transparent by considering the H_2^+ -ion (neglecting for the momentum spin-degrees of freedom and the identity of particles): The binding of this three body system can then be understood as the strong binding of the electron to one of the protons forming a group of 2 particles and the weak binding of the remaining proton by polarizing the neutral atom. Since no proton is distinguished, we could also start our considerations with the second proton forming a strongly bound group consisting of the electron and the second proton and the weakly bound first proton. In practice the electron will be considered as jumping resonantly from one configuration to the other so that a variational ansatz for the total wave function will consist of a linear combination of the two configuration. As interactions serve the basic two body potentials.

This simple example elucidates already the essential ideas of the RGM in nuclear physics. A solution for the total wave function is sought as linear combination of strongly bound substructures (groups of particles) times relative motion wave function and two-body interactions are employed. This idea of strongly bound substructures lead to the α -particle model of nuclei /BA 80/.

At first glance the RGM appears to be most suited to describe the relative motion of groups, i. e. collective motion or processes which are

dominated by compound nucleus formation. Due to the Pauli principle however, this is not so. This important point has been particular emphasized by Wildermuth /WI 79/. Below we will give an example which demonstrates that the RGM is capable of describing in one system with increasing energy compound nuclear processes and direct processes as well as the transition region. In a multichannel formulation elastic and inelastic scattering and reaction are described equally well. This flexibility of the RGM results from the following essential characteristics:

- 1) It is a microscopic formulation which takes explicitly substructures (clusters) into account.
- 2) The Pauli principle is fully accounted for by employing totally antisymmetric wave functions.
- 3) The center of mass motion is treated correctly.
- 4) Nucleon-nucleon potentials are used which reproduce the essential features of the two nucleon problem.
- 5) The nuclear bound-states, scattering and reaction problems are treated within the same framework utilizing one potential only.
- 6) The formulation is based on variational principles, hence, the results can be improved by expanding the model-space considered in the calculation.

Taken these points together we see that RGM is perfectly suited for studying examples where arbitrary composite nuclei interact with each other. Most formulations, however, are restricted to two-body dynamics only, see /HA 85/ for the contrary. It is unavoidable that the flexibility of the model raises the question of its technical feasibility at all. At the moment there exist essentially three different methods which allow numerical studies without further approximations and are applied to cases with more than one cluster decomposition: Two of them the complex-generator coordinate technique (CGCT) /TA 81/ and the Bargman transformation /SE 76, HQ 76/, employ single particle coordinates, whereas the third one, the refined resonating group model (RRGM) /HA 73/ works with Jacobi coordinates. Since by the use of single particle coordinates far developed shell model techniques are available for the calculation of many-particle matrix elements (ME), these methods are well suited for applications to heavier nuclei. On the other hand

in light nuclear system, where complicated internal wave functions are necessary to describe details of the reaction process the RRGM bears many advantages. For a connection between RRGM and Bargman transformations see /HA 77, ZA 81, SU 83/. I will in the sequel restrict my considerations mainly to the RGM because no concise manuscript exists till now for this method and in my opinion all essential ideas and advantages of the RGM can be most pedagogically presented in this framework, using simple examples. Furthermore this method in its basic approach is feasible only for few body system and is therefore more closely related to the topic of this school. On the other hand detailed manuscripts exist for the CGCT (see e. g. /TA 81/) and the Bargman transform /ZA 81, SU 83, FU 84/. Furthermore, the latter being mostly used in connection with the non-relativistic quark model additional degrees of freedom like color or antiparticles have to be introduced, such that the simple structure of the RGM is no more apparent.

In the next section we apply RGM to the bound and scattering potentials Problem, to show its differences and similarities and the connection to variational principles. The formulation of the RRGM is described in section 3. The classification and actual calculation of matrix elements is given in section 4. The essential point of all practical calculations the evaluation of the high dimensional spatial integrals is exploited in this section. In section 5 we discuss the notion of Pauli forbidden and partially Pauli forbidden states, the interpretation of RGM wave functions and the extraction of potentials. Some applications employing more realistic forces form the final section.

2. VARIATIONAL PRINCIPLES FOR THE POTENTIAL PROBLEM

2.1 A glimpse on the bound state problem

First we start with a brief review of the bound state problem in a potential model in order to set the notations and illustrate the method by a simple example, such that the differences to the potential scattering problem become evident.

The Hamiltonian for a spinless particle has the simple form

$$H = p^2/2M + V(R) = -\hbar^2 \Delta/2M + V(R) \quad (2.1)$$

where the potential $V(R)$ should be short ranged and nonsingular. For a

central potential V the wave function ψ can be expanded into partial waves

$$\psi(\underline{R}) = \sum_{LM} \psi_{LM}(\underline{R}) = \sum_{LM} u_L(R)/R Y_{LM}(\hat{\underline{R}}) \quad (2.2)$$

with real u_L . Here, as everywhere vectors are underlined and unit vectors carry additionally a hat $\hat{}$. This expansion leads to the well known radial Schrödinger equation

$$H_L u_L(R) = E u_L(R) \quad (2.3)$$

with

$$H_L = -\frac{\hbar^2}{2M} \left(\frac{d^2}{dr^2} - L(L+1)/R^2 \right) + V(R) = h_L + V(R) \quad (2.4)$$

Schrödinger's equation eq. (2.3) can be obtained from the variational principle

$$\delta \left[\int_0^\infty dR u_L(R) (H_L - E) u_L(R) \right] = 0 \quad (2.5)$$

Varying u_L , we have

$$\begin{aligned} \lim_{r \rightarrow \infty} \int_0^r dR [\delta u_L(R) (H_L - E) u_L(R) + u_L(R) (H_L - E) \delta u_L(R)] &= \\ = \lim_{r \rightarrow \infty} 2 \int_0^r dR \delta u_L(R) (H_L - E) u_L(R) &= 0 \end{aligned} \quad (2.6)$$

where H_L being selfadjoint on the square integrable functions u_L has been taken into account during shifting the action of the operators from δu_L to u_L . Hence, because δu_L is arbitrary, we obtain the required equation (2.3). In the many particle case, as we will see, the spatial integrals eq. (2.5) are only feasible for Gaussian functions. Therefore we will illustrate the convergence of the variational principle eq. (2.5) by choosing a potential $V(R)$ of Gaussian form and allow for the trial functions u_L linear combinations of Gaussians times R^L . To give some connection to later examples let us consider a proton and a neutron interacting via a central potential

$$V(R) = V_0 \exp(-b R^2) \quad (2.7)$$

where the parameters $V_0 = -66.327$ MeV and $b = 0.410125$ fm⁻² are chosen to reproduce the deuteron binding energy $E_D = -2.225$ MeV. In table 1

Number of Gaussians	width parameters from variation	kinetic energy	potential energy	binding energy
1	0.2055	12.783	-12.792	-0.009
2	0.5187 0.7382	11.105	-13.173	-2.068
3	0.7307 0.1831 0.03662	10.736	-12.948	-2.212
4	0.9099 0.3179 0.09036 0.02336	10.687	-12.911	-2.224
5	1.064 0.4625 0.1725 0.06090 0.01898	10.682	-12.907	-2.225

Table 1: Convergence study of the variational principle eq. (2.6) using various numbers of Gaussians for a pure central potential with parameters given below eq. (2.7).

We give the results of the non-linear variations for varying number of Gaussians. The convergence for the boundstate energy is rapid, already for two Gaussians the variations lie within 10 % of the numerical exact value. To achieve high precision, however, many terms are necessary. The approximate wavefunctions u are displayed in fig. 1 together with the numerically calculated one. We see that the approximate solutions wiggle around the exact one and fall off too fast with increasing R . Only for four and more Gaussians agree the two wave functions in the region displayed within the width of the lines drawn. From this simple example we can draw the conclusion, that we need about four Gaussian width parameters in order to reproduce a boundstate wave function up to 20 fm.

2.2 Potential scattering as variational problem

In this section we review briefly potential scattering following roughly along the lines of /HA 73/. The scattering wave function $u_l(R)$ is now no more normalized to unity but its asymptotic form consists of

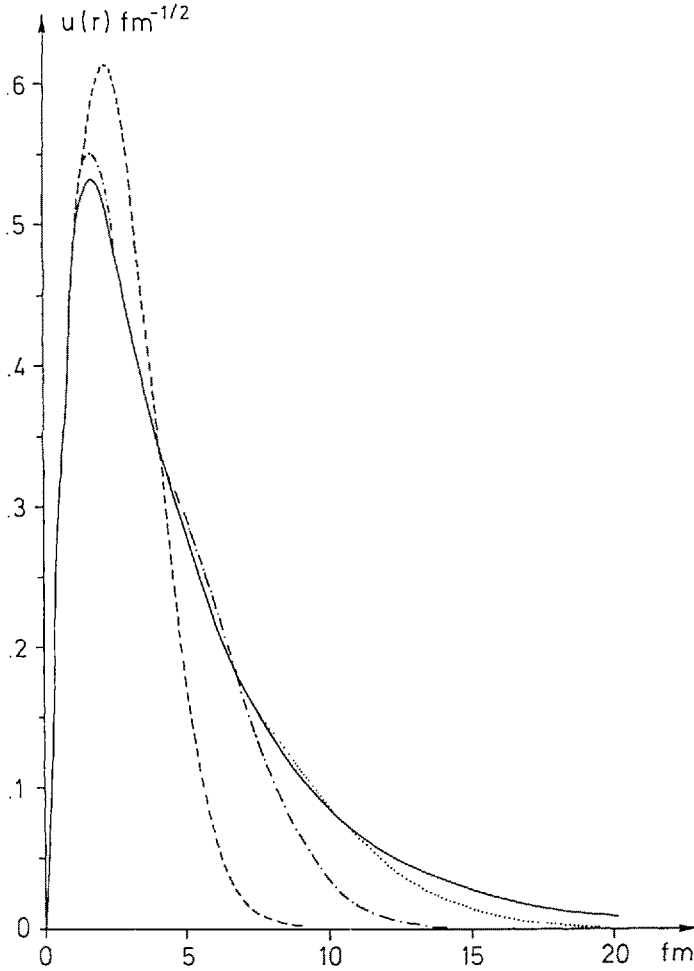


Fig. 1: Comparison of the exact wavefunction (full line) and the variational approximations using one Gaussian function (dashed line), two Gaussians (dashed-dotted line) and three Gaussians (dotted line). The approximations with four and more Gaussians are no more distinguishable from the full line.

a linear superposition of only two independent solutions of the free Hamiltonian h_L .

We will use here regular $F_L(R)$ and irregular solutions $G_L(R)$, because then all wave functions are real, such simplifying the numerical calculations. Even though the normalization of the total scattering wave function is irrelevant for determining physical quantities like cross sections etc., we normalize the total scattering wave function u_L in the following form

$$u_L(R) = \sqrt{M/\hbar^2 k} (F_L(R) + a \tilde{G}_L(R) + \sum_m b_{mL} X_{mL}(R)) \quad (2.9)$$

Where the momentum k is related to the energy by $E = \hbar^2 k^2 / 2M$ and for uncharged particles the regular and irregular wave functions are just the Riccati-Bessel functions /AB 64/ which are given for $L = 0$ as

$$F_0(R) = \sin kR \quad \text{and} \quad G_0(R) = \cos kR. \quad (2.10)$$

The X_{mL} are taken from a complete set of square integrable functions with $X_{mL}(R) \propto R^{L+1}$ for $R \rightarrow 0$.

In order $u_L(R)$ being regular, the irregular \tilde{G}_L has to be regularized such that

$$\tilde{G}_L(R) = T_L(R) G_L(R) \quad (2.11)$$

with

$$T_L(R) \propto R^{2L+1} \quad \text{for } R \rightarrow 0 \quad (2.12)$$

and

$$T_L(R) \rightarrow 1 \quad \text{for } R \rightarrow \infty \quad (2.12)$$

A convenient choice of the regularisation factor T_L is /HA 73/

$$T_L(R) = \sum_{i=2L+1}^{\infty} (\beta_0 R)^i / i! \exp(-\beta_0 R) = 1 - \sum_{i=0}^{2L} (\beta_0 R)^i / i! \exp(-\beta_0 R) \quad (2.13)$$

where both forms make the asymptotic values of T_L apparent for $R = 0$ and $R \rightarrow \infty$. The parameter β_0 is chosen in such a way that $T_L(R)$ approaches its asymptotic value of 1 just beyond the interaction region, an often used value is $\beta_0 = 1.1 \text{ fm}^{-1}$ /HO 84/.

The third term in eq. (2.9) has to account for the difference between the exact solution of the scattering problem and the ansatz determined by the asymptotic form of the solution. Furthermore in the region where T_L differs from 1 this term has to compensate the difference between \tilde{G}_L and G_L . With the standard choice of the parameter β_0 this means that this term is different from zero only in the interaction region and somewhat beyond, hence it can be well approximated even by a finite number of square integrable terms.

Since the scattering problem has a solution for every energy, the only

variational parameters left in eq. (2.9) are the (later) reactance matrix a and the expansion coefficients b_{mL} , after the set of square integrable functions X has been chosen. We will always choose the X_{mL} in the following form

$$X_{mL}(R) = R^{L+1} \exp(-\beta_m R^2) \quad (2.14)$$

The variational principle (2.5) will not lead to the Schrödinger equation, as we will show now.

Varying u_L as given in eq. (2.9) in eq. (2.5) we have

$$\lim_{r \rightarrow \infty} \int_0^r dR [\delta u_L(R)(H_L - E)u_L(R) + u_L(R)(H_L - E)\delta u_L(R)]. \quad (2.15)$$

In order to bring δu_L to the left of H_L we have to perform two partial integrations for the kinetic energy term, because on this scattering functions H_L is no more selfadjoint. Explicitely we find

$$\begin{aligned} \lim_{r \rightarrow \infty} \int_0^r dR [u_L(R) \left(-\frac{\hbar^2}{2M} \frac{d^2}{dR^2} \right) \delta u_L(R)] &= \\ &= \left(-\frac{\hbar^2}{2M} \right) \lim_{r \rightarrow \infty} \left\{ u_L(R) \frac{d}{dR} \delta u_L(R) \Big|_0^r - \delta u_L(R) \frac{d}{dR} u_L(R) \Big|_0^r + \int_0^r dR \delta u_L(R) \frac{d^2}{dR^2} u_L(R) \right\} \end{aligned} \quad (2.16)$$

Inserting (2.16) into eq. (2.15) we get

$$\begin{aligned} \delta \int_0^r dR u_L(R)(H_L - E)u_L(R) &= 2 \int_0^r dR \delta u_L(H_L - E)u_L - \\ &\quad - \frac{\hbar^2}{2M} \lim_{r \rightarrow \infty} \left(u_L \frac{d}{dR} \delta u_L - u_L \frac{d}{dR} u_L \right) \Big|_0^r \end{aligned} \quad (2.17)$$

The variational principle would give the desired Schrödinger equation, if the second term in eq. (2.17) would vanish. Since u_L is regular and all terms in eq. (2.9) are regular too, $u_L(0) = 0$ and $\delta u(0) = 0$. Thus the lower bound does not contribute. Noticing that the X_{mL} do not contribute to the upper bound, we find

$$\begin{aligned} -\frac{\hbar^2}{2M} \lim_{R \rightarrow \infty} (u_L(R) \frac{d}{dR} \delta u_L(R) - \delta u_L(R) \frac{d}{dR} u_L(R)) &= \\ = -\frac{\hbar^2}{2M} \frac{M}{\hbar k} \delta a_L \lim_{R \rightarrow \infty} F_L \frac{d}{dR} G_L - G_L \frac{d}{dR} F_L &= \\ = -\delta a_L / 2k \lim_{R \rightarrow \infty} \sin(kR - L\pi/2) \frac{d}{dR} \cos(kR - L\pi/2) - \cos(kR - L\pi/2) \cdot \\ \cdot \frac{d}{dR} \sin(kR - L\pi/2) = \delta a_L / 2 \end{aligned} \quad (2.18)$$

where the asymptotic form of the Bessel functions has been used. In case of charged particles, where F_L and G_L are Coulomb wavefunctions the Wronskian leads to the identical result.

In order to regain the Schrödinger equation we can therefore start from a modified variational principle

$$\delta \left[\int dR u_L(R) (H_L - E) u_L(R) - \frac{1}{2} a_L \right] = 0 \quad (2.19)$$

which is known as Kohn's variational principle. A much more rigorous and general derivation can be found in /GE 83/. Our normalization factor in eq. (2.9) resulted in the simple factor $\frac{1}{2}$ in eqs. (2.18) and (2.19).

Since F_L and G_L are solutions of the free Hamiltonian h_L to the correct energy it is easy to show, /HA 73/ that all integrals appearing in eq. (2.19) are of short range.

If we consider charged particles then h_L consists in addition to the kinetic energy also of the Coulomb term and the functions F_L and G_L are instead of Bessel functions Coulomb functions. All considerations, however, remain unchanged.

The solution of eq. (2.19) is not given here, because in the next section we discuss the solution of the variational equation in the general case, which is only slightly more complicated.

3. VARIATIONAL APPROACH TO MANY BODY SCATTERING

3.1 Variational equations and their solution

In this section we consider N nucleons which interact via nuclear and Coulomb forces. Two body forces are assumed throughout the text, but three-body forces are no principle problem, they can be treated along analogous lines as the two-body forces. Breakup channels into three or more fragments, however, pose a serious problem, because of the ansatz for the scattering wave function eq. (2.9), and will not be discussed in the following. In our presentation we follow along the lines of /HA 73, H0 84/.

With the assumption of two-body forces only the Hamiltonian of a N -

particle system is given by

$$H(1, \dots, N) = \sum_i T_i + \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (3.1)$$

The c.m. kinetic energy can be separated off, because of momentum conservation, yielding

$$\sum_{i=1}^N T_i = T_{CM} + \frac{1}{2mN} \sum_{i < j}^N (\underline{p}_i - \underline{p}_j)^2 \quad (3.2)$$

where m is the mass of the nucleons, assumed to be the same for neutrons and protons and \underline{p}_i is the momentum of nucleon i . Since we restrict our considerations to two-fragment channels only, the translationally invariant Hamiltonian H' can be decomposed into the internal Hamiltonian for both fragments and the relative motion part

$$\begin{aligned} H'(1, \dots, N) = & H_1(1, \dots, N_1) + H_2(N_1 + 1, \dots, N) + \\ & + T_{rel} + \sum_{\substack{i \in \{1, \dots, N_1\} \\ j \in \{N_1 + 1, \dots, N\}}} V_{ij} \end{aligned} \quad (3.3)$$

By adding and subtracting the point Coulomb interaction between the fragments $Z_1 Z_2 e^2 / R$ the potential term becomes shortranged, where R is the relative coordinate between the two fragments:

$$\begin{aligned} H'(1, \dots, N) = & H_1(1, \dots, N_1) + H_2(N_1 + 1, \dots, N) + \\ & + \left(\sum_{\substack{i \in \{1, \dots, N_1\} \\ j \in \{N_1 + 1, \dots, N\}}} V_{ij} - Z_1 Z_2 e^2 / R \right) \\ & + T_{rel} + Z_1 Z_2 e^2 / R \end{aligned} \quad (3.4)$$

Thus the translationally invariant part of the Hamiltonian is split into the internal Hamiltonians of the two fragments, the shortranged interaction of the fragments and the relative motion part of the two fragments with charges Z_1 and Z_2 . This decomposition now allows an ansatz for the total wave function ψ in the following form

$$\psi_1 = A \sum_{k=1}^{n_k} \psi_{kan}^k \psi_{rel}^{lk}, \quad (3.5)$$

where A denotes the antisymmetriser, n_k the numbers of channels, ψ_{kan}^k the channel wave function in channel k which will be described below

and ψ_{rel}^{1k} the relative motion wave function analogous to eq. (2.9)

$$\psi_{rel}^{1k}(R) = \delta_{1k} F_k(R) + a_{1k} G_k(R) + \sum_m b_{1km} X_{km}(R) \quad (3.6)$$

Here F_k and G_k are now the regular and regularised irregular Coulomb wave functions including the normalization factor of eq. (2.9). The index 1 on the total wave function ψ_1 is a reminder of the boundary condition chosen, namely regular waves only in channel 1. The sum k over channels runs over physical channels, open or closed, but it may also contain "distortion channels" which consist only of the square integrable part of eq. (3.6). Such distortion channels are especially needed if the number of physical channels is low, one or two, to allow for enough freedom for the variation.

The quantities a_{1k} and b_{1km} are the variational parameters, which are determined from Kohn's principle, analogously to eq. (2.19). As we saw in the previous section, the interference of regular and irregular free scattering waves results in a contribution of the endpoints of integration when switching over the operator $(H' - E)$ from $\delta\psi$ to ψ itself, hence Kohn's principle now reads /HA 73/.

$$\delta \langle \psi_1 | H' - E | \psi_1 \rangle - \frac{1}{2} a_{11} = 0. \quad (3.7)$$

The solution of the variational problem is described in the following. In order to simplify notation, we combine the individual terms of the relative motion wavefunction with the channel function such that

$$\psi_1 = A \left\{ \sum_k (f_k \delta_{k1} + a_{1k} g_k + \sum_m b_{1km} X_m') \right\} \quad (3.8)$$

The last term consists of square integrable functions only, hence, the Hamiltonian H' eq. (3.4) can be diagonalised in this function space. Let us assume, that this diagonalisation has been performed, then we can switch over to new square integrable functions Γ_ν with

$$\langle \Gamma_\nu | A \Gamma_\mu \rangle = \delta_{\nu\mu} \quad (3.9)$$

and

$$\langle \Gamma_\nu | H' | A \Gamma_\mu \rangle = e_\nu \delta_{\nu\mu}$$

Note: Since 1 and H' commute with the antisymmetriser A , it is enough to apply A on one wavefunction only, see also section 4.1. The total

wave function can now be represented as

$$\psi_1 = A \left\{ \sum_k (f_k \delta_{1k} + a_{1k} g_k) + \sum_m d_{1m} \Gamma_m \right\} \quad (3.10)$$

where now the variational parameters are a_{1k} and d_{1m} . Performing the variation, eq. (3.7) yields the following equations:

$$\langle g_k | \hat{H} | A f_1 \rangle + \sum_{k'} \langle g_k | \hat{H} | A g_{k'} \rangle a_{1k'} + \sum_m \langle g_k | \hat{H} | A \Gamma_m \rangle d_{1m} = 0 \quad (3.11a)$$

$$\langle \Gamma_m | \hat{H} | A f_1 \rangle + \sum_{k'} \langle \Gamma_m | \hat{H} | A g_{k'} \rangle a_{1k'} + \sum_{m'} \langle \Gamma_m | \hat{H} | A \Gamma_{m'} \rangle d_{1m'} = 0 \quad (3.11b)$$

where \hat{H} is an abbreviation of $H' - E$. Equation (3.11b) can be solved for $d_{1m'}$, taking eq. (3.9) into account

$$d_{1m} = (E - e_m)^{-1} (\langle \Gamma_m | \hat{H} | A f_1 \rangle + \sum_{k'} \langle \Gamma_m | \hat{H} | A g_{k'} \rangle a_{1k'}) \quad (3.12)$$

Defining the operator \tilde{H} as

$$\tilde{H} = \hat{H} - \sum_m \frac{\hat{H} | A \Gamma_m \rangle \langle \Gamma_m | \hat{H}}{e_m - E} \quad (3.13)$$

and inserting eq. (3.12) into (3.11a) yields

$$\sum_{k'} \langle g_k | \tilde{H} | A g_{k'} \rangle a_{1k'} = - \langle g_k | \tilde{H} | A f_1 \rangle \quad (3.14)$$

In obvious matrix notation eq. (3.14) reads

$$\langle G | \tilde{H} | G \rangle a^T = - \langle G | \tilde{H} | F \rangle \quad (3.15)$$

where a^T denotes the transposed matrix a . Equation (3.15) can be easily solved

$$a = - \langle G | \tilde{H} | F \rangle^T \langle G | \tilde{H} | G \rangle^{-1} \quad (3.16)$$

Now, if the matrix elements are known, the parameters of ψ_1 are determined in eq. (3.16) and consecutively in (3.12), hence, the total wave function is known.

Obviously, the reactance matrix a_{1k} in eq. (3.16) is not symmetric in the general case, therefore also the S-matrix computed from a_{1k} via

$$S = (1 + ia) (1 - ia)^{-1} \quad (3.17)$$

is not symmetric, thus violating time-reversal invariance. In general even unitarity is not guaranteed. To enforce unitarity we have to have a symmetric reactance matrix a . This goal is achieved by the so-called Kato correction /KA 51/ which can be understood most easily following /JO 71/.

Instead of the ansatz (3.10) we choose another boundary condition

$$\psi_l^i = A \left\{ \sum_k (a_{lk}^i f_k + \delta_{lk} g_k) + \sum_m d_{lm}^i \Gamma_m \right\} . \quad (3.18)$$

Following along the lines of eqs. (3.11) - (3.16) yields

$$a' = - \langle F | \tilde{H} | G \rangle^T \langle F | \tilde{H} | F \rangle^{-1} \quad (3.19)$$

again with an apparently unsymmetric a' . Since the special boundary condition chosen does not affect observables, we should have

$$a = a'^{-1} \quad (3.20)$$

Taking into account the properties of the channel wave function, discussed below, and the relative motion wave function it is easy to derive /JO 71/

$$\langle F | \tilde{H} | G \rangle = \langle G | \tilde{H} | F \rangle^T + \frac{1}{2} \mathbb{1} \quad (3.21)$$

by performing the partial integrations analogous to eq. (2.16) in order to switch the Hamiltonian \tilde{H} onto F . Inserting eq. (3.21) into (3.20) yields

$$- \langle G | \tilde{H} | F \rangle^T \langle G | \tilde{H} | G \rangle^{-1} = - \langle F | \tilde{H} | F \rangle (\langle G | \tilde{H} | F \rangle + \frac{1}{2} \mathbb{1})^{-1} \quad (3.22a)$$

or

$$\langle F | \tilde{H} | F \rangle = \langle G | \tilde{H} | F \rangle^T \langle G | \tilde{H} | G \rangle^{-1} (\langle G | \tilde{H} | F \rangle + \frac{1}{2} \mathbb{1}) \quad (3.22b)$$

or

$$\begin{aligned} - \langle G | \tilde{H} | F \rangle^T \langle G | \tilde{H} | G \rangle^{-1} &= a = \\ &= - 2 (\langle F | \tilde{H} | F \rangle - \langle G | \tilde{H} | F \rangle^T \langle G | \tilde{H} | G \rangle^{-1} \langle G | \tilde{H} | F \rangle) \end{aligned} \quad (3.22c)$$

where the last expression for a is obviously symmetric. This expression has been derived in /HA 73/ as second order correction and as stationary

condition in /GE 83/.

Employing eq. (3.17) we can now calculate cross sections etc., provided we are able to determine all matrix elements entering into eq. (3.22c). Before we discuss, how these matrix elements are calculated in praxi, we define the channel wave functions and discuss the existence of integrals.

3.2 Ansatz for the wave functions

The total wave function ψ_1 eq. (3.5) contains the channel functions ψ_{kan} and the relative motion wave function $\psi_{rel}(R)$. In the following we restrict our consideration to just one term of eq. (3.5) and study the action of the antisymmetriser A below. The channel function ψ_{kan} has the structure

$$\psi_{kan} = \left[Y_1(\hat{R}) R^{-1} \times [\phi_1^{J_1} \times \phi_2^{J_2}]^{S_c} \right]^J \quad (3.23)$$

Here $\phi_i^{J_i}$ denotes the translationally invariant wave function of fragment i ($i=1, 2$) with spin J_i . The individual spins J_1 and J_2 are coupled to the channel spin S_c . The orbital angular momentum l and S_c are coupled to total angular momentum J . The coupling is indicated by the square brackets. The vector \underline{R} denotes the relative vector between fragment 1 and 2 in case of a scattering wave function and the corresponding Jacobi coordinate in case of a bound state wave function. In the latter case the coupling to total J can be omitted.

The individual fragment wave function consist of the spatial function X and the spin (isospin) function Ξ , e. g.

$$\phi_1^{J_1} = \sum_{l_I, S, m} \left[C_{m}^{l_I L S} X_m^{l_I(\underline{\rho}) \Xi^{S, T}} \right]^{J_1} \quad (3.24)$$

where l_I denotes the set of internal orbital angular momenta of fragments consisting of more than one cluster. We use the expression "cluster" only for groups of particles without internal orbital angular momenta, i. e. the largest cluster can contain only 4 particles, two protons and two neutrons with opposite spin projections. The spin (-isospin) functions Ξ are coupled to total spin S and may be coupled to good isospin. For a fragment consisting of n_c clusters the coefficients $C_m^{l_I L S}$ include the Clebsch-Gordan coefficients for the coupling of the orbital angular momenta $l_1, l_2, \dots, l_{n_c-1}$ to total orbital angular

momentum L , the coupling of the spin (and isospin) to S (and T) and additional coefficients, which allow a superposition of different radial dependencies. The spatial function χ_m^{1I} is constructed from cluster internal functions $\chi_{m,int}$ and cluster relative functions $\chi_{m,rel}$ in the form

$$\chi_m^{1I} = \left(\prod_{h=1}^{n_c} \chi_{m,h,int} \right) \left(\prod_{k=1}^{n_c-1} \chi_{m,k,rel}^{1k} \right) \quad (3.25)$$

where the internal functions consist of a single Gaussian function

$$\chi_{m,h,int} = \exp \left(-\beta_{mh} \sum_{i < j}^{n_h} (\underline{r}_i - \underline{r}_j)^2 / n_h \right) \quad (3.26)$$

with n_h denoting the number of nucleons (≤ 4) inside cluster h , which has a width β_{mh} . In case of the cluster containing just one nucleon $\chi_{m,h,int} \equiv 1$. The cluster relative functions $\chi_{m,k,rel}^{1k}$ contain in addition to the Gaussian-function solid spherical harmonics y_{1k} /ED 64/

$$\chi_{m,k,rel}^{1k} = \exp \left(-\gamma_{mk} \rho_k^2 \right) y_{1k}(\underline{\rho}_k) \quad (3.27)$$

where ρ_k denotes the Jacobi coordinate between cluster $k+1$ and the center-of-mass of the cluster 1 to k , see fig. 2.

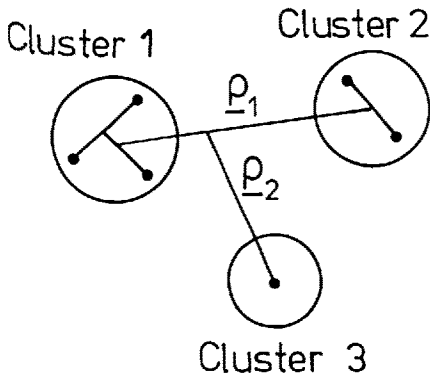


Fig. 2:
Schematic illustration of the intercluster coordinates ρ used in eq. (3.27).

The wavefunctions ϕ_i^{Ji} are determined from the Ritz variational principle analogous to eq. (2.5) once the fragmentation and number of radial functions has been chosen. Therefore, in the function space chosen ϕ_i^{Ji} is most deeply bound with e. g. for fragment 1

$$\langle \phi_1^{J1} | H'(1, \dots, N_1) | A_1 \phi_1^{J1} \rangle = E_1 \langle \phi_1^{J1} | A \phi_1^{J1} \rangle \quad (3.28)$$

where A_1 is the antisymmetriser for the first N_1 nucleons. Denoting analogously the antisymmetriser for the remaining group of $N - N_1$ nucleons by A_2 , we can write the total antisymmetriser as

$$A = A_3 A_1 A_2 = \sum_{P_3} (-1)^{P_3} P_3 A_1 A_2 \quad (3.29)$$

where the sum P_3 runs over all permutations which exchange particles between the two fragments, including the identity.

In order to show that the solution of the variational problem is more than just a formal one, we must prove that the functional of eq. (3.7) exists. If we take the kinetic energy ϵ_k in channel k to be

$$\epsilon_k = E - E_{1,k} - E_{2,k} \quad (3.30)$$

then the Hamiltonian eq. (3.4) can be decomposed as

$$\begin{aligned} H'(1, \dots, N) - E &= (H_1(1, \dots, N_1) - E_{1,k}) + (H_2(N_1 + 1, \dots, N) - E_{2,k}) + \\ &+ \left(\sum_{\substack{i \in \{1, \dots, N_1\} \\ j \in \{N_1 + 1, \dots, N\}}} V_{ij} - Z_1 Z_2 e^2 / R \right) + \\ &+ T_{rel} + Z_1 Z_2 e^2 / R - \epsilon_k \end{aligned} \quad (3.31)$$

All terms in eq. (3.7) which contain only square integrable functions cannot lead to divergent integrals. The same is true for all terms in which the functions of channels with different fragmentations are connected. Furthermore, all integrals involving an exchange of nucleons between the fragments, i. e. $P_3 \neq 1$, are of short range. Hence, the only possibly dangerous integrals involve identical fragmentations in bra and ket of the matrix elements and P_3 being the identity. Under these circumstances the first line of eq. (3.31) contributes zero because the internal functions ϕ_i^j are solutions to just the energies $E_{i,k}$, see eq. (3.28). The second line results in a short-ranged integral by construction. If and only if, the Coulomb function F_k and G_k in eq. (3.6) are chosen as eigenfunctions of the last line of (3.31), the related integrals are finite. This implies that the threshold energies are completely fixed by the binding energies of the fragments and therefore one has no possibility to adjust those energies.

Since we have now convinced ourselves that all integrals are short-

ranged, we can expand within the relevant region the regular and regularised irregular Coulomb function in terms of Gaussian functions, e. g. the square integrable function X of eq. (3.6). By this expansion we are left with integrals of the Hamiltonian or unity between translationally invariant wavefunctions consisting besides the spin-isospin part only of linear combinations of Gaussians and solid spherical harmonics.

In the next section we will describe how to calculate such a matrix-element.

4. EVALUATION OF THE MATRIX ELEMENTS

4.1 Reduction to reduced matrix elements

For the calculation of the matrix elements, we have to apply the anti-symmetriser A onto the wavefunctions in bra and ket as

$$\langle A \psi^{J'M'} | \sum_{i < j} w_{ij} | A \psi^{JM} \rangle \quad (4.1)$$

where $\sum w_{ij}$ is either the Hamilton operator or just the unit operator. Since the operator A commutes with the symmetric operator $\sum w_{ij}$ and we are calculating expectation values only, we can reduce the expression (4.1) to

$$ME = \langle \psi^{J'M'} | A \sum_{i < j} w_{ij} | \psi^{JM} \rangle \quad (4.2)$$

by using the proportionality between A^2 and A . For the further calculation we decompose A into the sum over all permutations acting on spatial, spin and isospin coordinates

$$A = \sum_P (-1)^P P \quad (4.3)$$

For each permutation eq. (4.2) has to be calculated. Here ψ^{JM} denotes a single term of the total wavefunction ψ eqs. (3.5) and (3.6) allowing for the various fragmentations of the channels, the possible different components of the internal functions, eqs. (3.23) and (3.24), and the various square integrable functions X in eq. (3.6). Because of the rotational invariance of the Hamiltonian the operator $\sum w_{ij}$ can be decomposed into a product of orbital and spin space spherical tensors /ED 64/

$$\sum_{i < j} w_{ij} = \sum_{i < j} \sum_{kq} (-1)^q w_{ij}^0(k, q) w_{ij}^S(k, -q) \quad (4.4)$$

where k denotes the rank of the interaction, e. g. $k=2$ for the tensor potential.

The wavefunction ψ^{JM} consists of orbital and spin-isospin part according to

$$\psi^{JM} = \sum_{\alpha} c_{\alpha}^{LSJ} (Lm S\sigma | JM) \psi_{\alpha}^{Lm}(\text{space}) \psi_{\alpha}^{S\sigma}(\text{spin}) \quad (4.5)$$

where the Clebsch-Gordan coefficient $(Lm S\sigma | JM)$ explicitly gives the coupling of total orbital angular momentum L and total spin S to J . The index α is a short notation of all other quantum numbers, e. g. the fragmentation. Using Racah algebra we find for fixed i, j and k for eq. (4.2)

$$\begin{aligned} M_{ijk} &= \sum_P \langle \psi^{J'M'} | \sum_q (-1)^P (-1)^q P w_{ij}^0(kq) w_{ij}^S(kq) | \psi^{JM} \rangle \\ &= \delta_{JJ'} \delta_{MM'} \sum_{\alpha\alpha'} \sum_P (c_{\alpha}^{L'S'J})^* c_{\alpha}^{LSJ} (-1)^P (-1)^{L+2S+S'-J} \left\{ \begin{matrix} S & L & J \\ L' & S' & k \end{matrix} \right\} \\ &\quad \langle L'\alpha' || P w_{ij}^0(k) || L\alpha \rangle \langle S'\alpha' || P w_{ij}^S(k) || S\alpha \rangle \end{aligned} \quad (4.6)$$

where $\left\{ \begin{matrix} S & L & J \\ L' & S' & k \end{matrix} \right\}$ is a 6j-coefficient /ED 64/.

4.2 Calculation and classification of the spin-isospin matrix elements

According to eq. (4.6) we have to calculate reduced spin matrix elements which is done by using Wigner-Eckart theorem

$$\begin{aligned} \langle S'\alpha' || P w_{ij}^S(k) || S\alpha \rangle &= (2S'+1)^{1/2} \langle S'S'\alpha' | P w_{ij}^S(k, S'-S) | SS\alpha \rangle / \\ &\quad (SSk S' - S | S'S') \end{aligned} \quad (4.7)$$

We use here maximal projections of the spin functions so the ME is different from zero, if the triangular conditions are fulfilled at all.

The coupled spinfunctions $|SS\alpha\rangle$ can be decomposed into linear combinations of products of elementary single particle spin function by using again Clebsch-Gordan coefficients. Analogously consists w_{ij}^S of products of the isospin operators 1 resp. $\tau_i \cdot \tau_j$ with the spin operators 1 (for norm and central potential), $\underline{\sigma}_i \cdot \underline{\sigma}_j$ (for central poten-

tial), $(\underline{\sigma}_i + \underline{\sigma}_j)_q$ spherical component q (for spin-orbit potential) and $\sigma_{iq} \sigma_{jq}$, (for the tensor potential). These operators acting on product wave functions again give product wavefunctions. The permutation P can be easily applied onto this product and the ME can be easily evaluated. Since usually many of these matrix elements vanish, it is more economic to start from product functions in bra and ket and determine all permutations P which give a ME different from zero, for details see /HA 73, HO 84/. To find the reduced matrix elements (4.7) itself, only the summation over the known Clebsch-Gordan coefficients have to be performed.

As will be shown below, the calculation of the spatial matrix elements is much more complicated than that of the spin matrix elements. Therefore the symmetry of the spatial wavefunctions is utilized. Here the cluster decomposition plays the essential role. From the ansatz for the internal coordinate space wave functions eq. (3.25) to (3.27) it is evident that the function in coordinate space is symmetric under exchange of nucleons inside of clusters, but not if particles are exchanged beyond cluster boundaries. Hence, different permutations may yield identical orbital matrix elements.

In order to exploit this symmetry one considers instead of the symmetric group S_n itself subgroups $S_{n_1} \times S_{n_2} \times \dots$ with $\sum n_i = N$ in bra and ket, where n_i is the number of nucleons in cluster i /SE 75/. The group S_n is decomposed into double cosets of these subgroups, and each double coset can be characterised uniquely by one permutation. Restricting, for the moment, our considerations to the norm, where $w_{ij} = 1$, we find for permutations belonging to one double coset always the same orbital ME. Therefore, the known spin MEs belonging to one double coset can be summed up, including the sign of the permutation. This allows to reduce the sum over all permutations in eq. (4.6) appreciably to a sum over double cosets only

$$M_{ijk} = \delta_{JJ'} \delta_{MM'} \sum_{\alpha} (C_{\alpha}^{L'S'J})^* C_{\alpha}^{L S J} (-1)^{L+2S+S'-J} \begin{Bmatrix} S & L & J \\ L' & S' & k \end{Bmatrix} \sum_{dc} \langle L' \alpha' | | P_{dc} w_{ij}^0(k) | | L \alpha \rangle C_{dc}^{SS' \alpha' ij} \quad (4.8)$$

where $C_{dc}^{SS' \alpha' ij}$ contains the sum over spin MEs and P_{dc} is any permutation representing the double coset dc . If the ME contains an interaction $w_{ij} \neq 1$ one has also to mark the interacting particles i and j and to extend the double coset decomposition.

In the following we will not elaborate on a general treatise on double cosets, this can be found in /SE 75, LU 81/, but rather give an illustrative example /HO 84/. Let us consider the ${}^7\text{Be}$ nucleus, which can be described very well in a fragmentation ${}^4\text{He}$ and ${}^3\text{He}$, but small components of a fragmentation ${}^6\text{Li}$ and p allow to reproduce experimental data better /ME 86/, see also final section.

The decomposition into double cosets can be illustrated by symbols of matrix form, which are called dc-symbols /SE 75/. In the ${}^7\text{Be}$ case we have for example a decomposition of the S_7 into $S_4 \times S_3$, for the main component of the wave function, and $S_4 \times S_2 \times S_1$ for the small component. Note that the ${}^6\text{Li}$, containing 6 nucleons, has to contain at least 2 clusters, the main component being ${}^4\text{He} - {}^2\text{H}$ (for further details see /ME 86/).

	S_4	S_3
S_4	3	1
S_2		2
S_1	1	

In the different sites of the scheme we have entered the number of particles which are exchanged by the permutation from the cluster given on the left side into the cluster stated above. The sum of one row (column) is always the number of nucleons in that cluster, as can be seen in the above example. The second row illustrates that 2 particles from the ${}^2\text{H}$ cluster are exchanged into the ${}^3\text{He}$ -cluster.

A dc-symbol can be associated with each permutation and permutations having the same dc-symbol belong to the same double coset /SE 75/. On the other hand, a permutation representing the double coset can be constructed uniquely from the dc-symbol. To achieve this we write the digits 1 to N rowwise into the dc-symbol, as many digits as indicated per site, and then read this scheme columnwise. If one writes the digits found by this procedure below the digits 1 to N in natural order one finds a permutation representing the double coset. In our example this will read

	S_4	S_3
S_4	123	4
S_2		56
S_1	7	

$$= \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 2 & 3 & 7 & 4 & 5 & 6 \end{pmatrix} = p_{dc}$$

One has to discriminate the orbital MEs, in addition to which particles are interacting. For this we mark the permuted digit of the interacting particles with a point. For two body-interactions we find for interacting particles 4 and 6 the digits in our above example.

$$7 (= P_{dc}(4)) \quad \text{and} \quad 5 (= P_{dc}(6))$$

	S_4	S_3
S_4	123	4
S_2		5 [•] 6
S_1	7 [•]	

The group configurations indicated are often omitted for convenience. Thus we arrived at a new classification scheme for matrix elements of any two-body interaction in terms of 2-point dc-symbols. The example tells us, that also an interaction between particle 4 and 7 would yield the same coordinate space ME. Therefore one adds up all spin ME belonging to the same 2-point dc-symbol. Analogously the sum over dc in eq. (4.8) runs over all 2-point dc symbols in case of an interaction. Extending this classification scheme to one-body or more-body interactions is straight forward. It remains only to calculate the ME in coordinate space, which will be described in the following subsection.

4.3 Evaluation of the orbital matrix elements

The reduced MEs of eq. (4.8) are converted into usual integrals analogous to eq. (4.7). Since the coupling scheme of the various orbital angular momenta just introduces trivial linear combinations, we disregard this complication in the sequel and start with the bare orbital functions, which are for the right hand side of the ME (marked by the index r) of the structure

$$|L_r \alpha\rangle = \prod_{i=1}^{N-1} \exp(-\beta_i \underline{s}_i^r \cdot \underline{s}_i^r) \prod_{j=1}^{n_{cr}} y_{1_j m_j}(\underline{s}_{N-n_{cr}+j}^r) \quad (4.9)$$

where the numbering of the Jacobian coordinates \underline{s}_i starts with the internal coordinates, see fig. 3, and the single particle coordinates of eq. (3.26) have been eliminated in favour of the Jacobians. Note, that because of translational invariance the c. m. coordinate, proportional to \underline{s}_N , is absent in eq. (4.9); the number of cluster is denoted by n_{cr} . The function on the left hand side $|L_r \alpha\rangle$ can be expressed

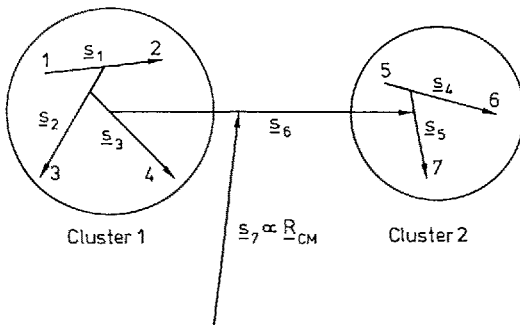


Fig. 3:
Schematic diagram illustrating the numbering of the Jacobi coordinates of eq. (4.9) for a cluster decomposition into 4 and 3 particles. Note, that the arrows shown are only proportional to the Jacobi vectors.

analogously by Jacobian coordinates of the left hand side (index 1), which will be different from the right hand side in the general case. Starting from eq. (4.8) we want to show how to evaluate a ME of the type

$$J_{L_1\alpha', L_r\alpha}^{ij}(P_{dc}) = \langle L_1\alpha' | P_{dc} w_{ij}^0(k) | L_r\alpha \rangle \quad (4.10)$$

The operators w_{ij} contain coordinates in the form of eq. (4.9) or in addition to that also differential operators may occur. In order to keep the presentation as transparent as possible, we restrict our considerations in the following to the norm and refer for the other operators to the literature /HA 70, HO 84/.

Choosing the Jacobian coordinates of the left hand side as independent variables and suppressing their index 1 in the following we can express the ME eq. (4.10) by

$$\begin{aligned} J_{L_1\alpha', L_r\alpha}^{ij}(P_{dc}) &= \int d\underline{s}_1 \dots d\underline{s}_{N-1} \exp \left(-\sum_{\mu\mu'} \rho_{\mu\mu'}(P_{dc}) \underline{s}_\mu \cdot \underline{s}_{\mu'} \right) \prod_{n=1}^Z \gamma_{L_n M_n}(\underline{Q}_n) = \\ &= \Gamma_{L_1 M_1 \dots L_Z M_Z} \end{aligned} \quad (4.11)$$

Since in the norm no particles interact, we have suppressed the indices i and j on the symbol Γ . The coefficients $\rho_{\mu\mu'}$ result from expressing the Jacobians of the r. h. s. by those of the left hand side, applying the permutation P_{dc} first. The \underline{Q}_n vectors are the intercluster coordinates after applying P_{dc} to the r. h. s. and can be expressed as linear combinations of the Jacobians \underline{s} . In case of an interaction w_{ij}^0 , its radial dependence in Gaussian form has to be included into ρ . See for an example of other radial dependencies in the Appendix A. The combined number Z of orbital angular momenta is

$$Z = n_{cl} - 1 + n_{cr} - 1 + n_w \quad (4.12)$$

where $n_w = 1$ for the tensor interaction and $n_w = 0$ otherwise. Except for the solid spherical harmonics, the ME in eq. (4.11) is just a multidimensional Gaussian integral, which is straightforward to evaluate by bringing $\rho_{\mu\mu'}$ to diagonal form. In order to utilize this procedure we introduce the generating function for the spherical harmonics /R0 57/

$$(\underline{b} \cdot \underline{r})^L = b^L \sum_{m=-L}^L C_{Lm} b^{-m} y_{Lm}(\underline{r}) \quad (4.13)$$

employing the vector $\underline{b} = (1 - b^2, i(1 + b^2), -2b)$, with the property $\underline{b} \cdot \underline{b} = 0$. The coefficient C_{Lm} are given by

$$C_{Lm} = (-2)^L L! (4\pi / ((2L+1)(L-m)!(L+m)!))^{1/2} \quad (4.14)$$

Instead of eq. (4.11) we now consider the generating integral

$$I(a_1 b_1 \dots a_z b_z) = \int d\underline{s}_1 \dots d\underline{s}_{N-1} \exp(-\sum_{\mu\mu'} \rho_{\mu\mu'} \underline{s}_\mu \cdot \underline{s}_{\mu'} + \sum_{n=1}^Z a_n \underline{b}_n \cdot \underline{Q}_n) \quad (4.15)$$

Expanding the expression $\exp(\sum a_n \underline{b}_n \cdot \underline{Q}_n)$ into a power series in a_n and \underline{b}_n and taking eq. (4.13) into account we relate the generating integral to the desired ones

$$I(a_1 b_1 \dots a_z b_z) = \sum_{l_1 m_1 \dots l_z m_z} \left(\prod_{n=1}^Z C_{l_n m_n} / l_n! \right) a_1^{l_1} b_1^{l_1 - m_1} \dots a_z^{l_z} b_z^{l_z - m_z} \quad (4.16)$$

On the other hand the generating integral eq. (4.15) can be evaluated explicitly and afterwards expanded into a power series. To accomplish this we first transform the expression $\rho_{\mu\mu'} \underline{s}_\mu \cdot \underline{s}_{\mu'}$ onto diagonal form by

$$\underline{s}_\mu = \sum_{\lambda=\mu}^{N-1} T_{\mu\lambda} \underline{t}_\lambda \quad \text{with } T_{\lambda\lambda} = 1 \quad (4.17)$$

which yields

$$\sum_{\mu\mu'} \rho_{\mu\mu'} \underline{s}_\mu \cdot \underline{s}_{\mu'} = \sum_{\lambda} B_{\lambda} \underline{t}_{\lambda}^2 \quad (4.18)$$

and

$$\underline{Q}_n = \sum_{\mu} P_{n\mu} \underline{t}_{\mu} \quad (4.19)$$

Inserting eq. (4.18) and (4.19) reduces eq. (4.15) to the form

$$I(a_1 b_1 \dots a_z b_z) = \int dt_1 \dots dt_{N-1} \exp(-\sum_{\lambda} (\beta_{\lambda} t_{\lambda}^2 - \sum_n P_{n\lambda} a_n \cdot b_n \cdot t_{\lambda})) \quad (4.20)$$

where the condition on $T_{\lambda\lambda}$ has been utilized. Employing the method of completing squares the integral amounts to

$$I(a_1 b_1 \dots a_z b_z) = \left(\prod_{r=1}^{N-1} (\pi/\beta_r) \right)^{3/2} \exp\left(\frac{1}{4} \sum_{n,n'} \sigma_{nn'} a_n a_{n'} \cdot b_n \cdot b_{n'}\right) \quad (4.21)$$

where we defined

$$\sigma_{nn'} = 2 \sum_{\lambda} P_{n\lambda} P_{n'\lambda} / \beta_{\lambda} \quad (4.22)$$

Computing the scalar product $b_n \cdot b_{n'}$, and restricting the summation over n and n' allows to reduce the exponent in eq. (4.21) to

$$\sum_{n>n'} \sigma_{nn'} a_n a_{n'} (b_n b_{n'} - \frac{1}{2} (b_n^2 + b_{n'}^2)) \quad (4.23)$$

Expanding the exponential in eq. (4.21) into a power series and collecting terms in the form of eq. (4.16) yields the final result /HA 70, HQ 84/

$$\Gamma_{l_1 m_1 \dots l_z m_z} = \left(\prod_{r=1}^{N-1} (\pi/\beta_r) \right)^{3/2} \left(\prod_{j=1}^Z l_j! / C_l j^{m_j} \right) \sum_{g_{nn'}, h_{nn'}, k_{nn'}} (-1/2)^{h_{nn'} + k_{nn'}} \prod_{n>n'} \sigma_{nn'}^{g_{nn'} + h_{nn'} + k_{nn'}} / (g_{nn'}! h_{nn'}! k_{nn'}!) \quad (4.24)$$

The sums $g_{nn'}$, $h_{nn'}$, and $k_{nn'}$ run over all possible combinations of nonnegative integers, which fulfill the following relations:

$$2 \sum_{n>n'} (g_{nn'} + h_{nn'} + k_{nn'}) = \sum_{j=1}^Z l_j \quad (4.25a)$$

$$\sum_{n \neq n'} (g_{nn'} + h_{nn'} + k_{nn'} + g_{n'n} + h_{n'n} + k_{n'n}) = l_n \quad (4.25b)$$

$$\sum_{n \neq n'} (h_{n'n} - h_{nn'} - k_{n'n} + k_{nn'}) = m_n \quad (4.25c)$$

In these relations $g_{nn'} = h_{nn'} = k_{nn'} = 0$ if $n < n'$. The eqs. (4.25) allow in the case of more than two clusters in bra or ket many solutions, which have to be found by trial and error. A very efficient computer program, based on a scheme given in /ST 70/, accomplishes this task.

We are now in the position to calculate the norm matrix element from

eq. (4.24), with the help of eqs. (4.14), (4.18), (4.19), (4.22) and (4.25). In addition to that the ME of the central potential is also given by eq. (4.25), proviso the radial dependence of the force has been included into $\rho_{\mu\mu}$ of eq. (4.11), which then modifies accordingly the elements β and σ_{nn} . Analogous considerations apply for the tensor force except that the number of orbital angular momenta has to be increased by one. With the relation /ED 60/

$$4\pi/(2l+1) \sum_{m=-l}^l (-1)^m y_{lm}(\underline{r}) y_{l-m}(\underline{r}) = r^{2l} \quad (4.26)$$

one can now utilize more complicated orbital wave functions which may then consist of Gaussian times solid spherical harmonics times polynomials in r^2 at the expense of two additional angular momenta for each monomial in eq. (4.9) and following. The calculation of other operators follows along the lines of eq. (4.9) to (4.25). The results can always be expressed by normintegrals times factors which can be easily calculated. The explicit expressions can be found in the literature for the kinetic energy /HH 70, H0 84/, the spin-orbit potential /H0 84/ and for electromagnetic transition operators /ME 86/.

The method described above can only be efficiently applied, if the radial dependence is given in terms of Gaussians. Besides the many effective nucleon-nucleon potentials given in Gaussian form, there are two realistic NN-potentials /EI 71, KE 86/ with full operator structure but as radial dependence only sums of Gaussians. These potentials reproduce the NN data up to the pion threshold. Other operators can be expressed in terms of Gaussians /BU 85/, e. g. the $1/r$ -dependence of the Coulomb potential may be written as

$$1/r = 2\sqrt{\beta/\pi} \int_0^\infty dk \exp(-k^2\beta r^2) \quad (4.27)$$

Which is again of Gaussian form and can be treated by the above method. Since in the framework of the RRGm the Coulomb force can be treated exactly contrary to many other approaches, we derive the ME in the Appendix.

With the methods described till now, we can evaluate all matrix elements and thus attack any problem. Before applying these methods to actual cases we study in the following section general properties of the RGM.

5. RGM WAVE FUNCTION AND EQUIVALENT LOCAL POTENTIALS

5.1 Interpretation of the RGM wave function

In section 3 the variational equations were solved for the reactance matrix a , which is the only observable quantity for scattering systems. If we are, however, interested in properties of bound states or in electromagnetic transitions then we need the variational wavefunction itself, i. e. we need the coefficients d_{lm} in eq. (3.10) which were eliminated by eq. (3.12). Let us for simplicity concentrate on the bound state problem, since transitions are only slightly more complicated and give no new inside.

The many body bound state problem can be solved with the variational procedure described in section 3, by reducing the ansatz for the wave function eq. (3.8) to square integrable functions only

$$\psi = A \sum_m b_m X_m \quad (5.1)$$

In order to have a transparent notation we number the functions consecutively and specify no more the channel k from which they originate. Since we restricted our considerations to the bound state problem, we can start from the analogue of eq. (2.5) in the many body case. Performing the variation we find

$$\sum_j (H_{ij} - E N_{ij}) b_j = 0 \quad (5.2)$$

with

$$H_{ij} = \langle X_i | H | A X_j \rangle \quad (5.3a)$$

and

$$N_{ij} = \langle X_i | A | X_j \rangle \quad (5.3b)$$

Noting that the matrix N_{ij} is positive semi-definite standard methods to solve the general eigenvalue problem /W1 65/ eq. (5.2) can be applied.

The symmetric matrix N can be diagonalised by an orthogonal matrix B yielding a positive diagonal matrix. For the moment we exclude the possibility of a zero eigenvalue, but return to this point later on. Thus we can write the matrix N as

$$N = B^T D B \quad (5.4)$$

With this expression we find from eq. (5.2)

$$H - EN = B^T D (D^{-1} B H B^T D^{-1} - E) D B = B^T D (P - E) D B \quad (5.5)$$

The symmetric matrix P has a complete set of eigenvectors z_i which may be taken orthogonal. We therefore have

$$P z_i = e_i z_i \quad (5.6)$$

giving

$$H(B^T D^{-1} z_i) = e_i B^T D z_i = e_i B^T D D B B^T D^{-1} z_i = e_i N(B^T D^{-1} z_i) \quad (5.7)$$

Hence $x_i = B^T D^{-1} z_i$ is an eigenvector of the generalised eigenvalue problem eq. (5.2), which fulfills the relations (3.9). We mention in passing that all solutions e_i of eq. (5.2) which are below the first threshold energy E_{th} are an upper bound for the energy of bound states. The energies $e_i > E_{th}$ have no intuitive physical meaning and cannot be interpreted as resonances /HA 73/.

Equation (5.2) is the matrix version of the standard RGM equation using integrals kernels /TA 81/

$$\{(\mathcal{H}(\underline{R}', \underline{R}) - E \mathcal{N}(\underline{R}', \underline{R})) F(\underline{R}) d\underline{R} = 0 \quad (5.8)$$

This is obviously not of the usual form of the Schrödinger equation, therefore we cannot interpret $F(R)$ as probability amplitude, but rather $N^{1/2} F(R)$. This suggests by analogy that we can interpret $N^{1/2} x_i$ straightforwardly as probability amplitudes too. Because our basis functions x_m are neither normalised nor orthogonal $N^{1/2}$ is not just DB , but some care has to be taken in defining $N^{1/2}$ /BU 86/.

The RRGM differs in another point again from standard RGM: In case of equal width parameters for both fragments in the internal wave function eq. (3.26) and (3.27) we may have a zero norm eigenvalue.

In the standard RGM these redundant states /TA 81/ are a stringent test of the correct calculation of the norm and hamiltonian kernels. In the RRGM, however, we have to avoid such states. Since we have to divide by the square root of the norm eigenvalues during the transformation of H the standard routines for solving the general eigenvalue problem would fail. The redundant states are also called Pauli forbidden states. In

case of different width parameters in both fragments, a zero norm eigenvalue is no more possible, but norm eigenvalues might be small. The corresponding eigenvectors are then often called almost Pauli forbidden state.

The existence of these Pauli forbidden (PV) states obviously prevents the direct physical interpretation of the solutions of eq. (5.2), because inside the range in which the PV are different from zero the solution is arbitrary. With the factor $N^{1/2}$, however, these arbitrary components are projected onto zero. The number of PV can be easily determined by considering the corresponding oscillator shell model states /H0 77/, examples are given in /TA 81/. On the other side these PV form the basis for the orthogonality condition model /SA 69/.

The RGM wave functions contain a further source of arbitrariness. In case of coupled channels we may consider different fragmentations, e.g. in the $A=6$ case ${}^4\text{He} + d$ and ${}^3\text{He} + {}^3\text{H}$. Since the resulting channel wave functions eq. (3.23) may be non-orthogonal, we cannot answer the question of the admixture probability in the total wave function uniquely. This can be done only if solely orthogonal channels are taken into account, which can be done by applying some orthogonalisation procedure onto the non-orthogonal channels /SC 85/. These channels, however, do no more consist of the physical particles only. Compared to the full microscopic wave function eq. (3.5) these orthogonal channels give no deeper physical insight. Considering, however, only the relative motion part, the orthogonalised channel approach allows to draw well defined conclusions, for an example see /SP 86/.

5.2 Extraction of equivalent local potentials

As we have shown in the previous sections, the RGM provides an approximate solution of the relative motion wave function of two complex fragments with proper antisymmetrisation taken into account. Because of the exchange terms, P_3 of eq. (3.29) being different from the identity, the resulting kernels in eq. (5.8) are non-local.

Since local potentials are much easier to handle, one searches for such a local potential, containing the antisymmetrisation proper, which can be applied in much cruder reaction models like DWBA. Because of the problem associated with the non-orthogonality of channels discussed in the previous section, I restrict in the following my considerations to

the single channel case only, see, however, /YA 85/ for the coupled channel approach.

Two different methods are used to define such a local potential. The easiest to understand is based on the potential Schrödinger equation eq. (2.3). Since we are now left with a function of the relative coordinate only, which we know from eq. (5.2) or (3.8) together with eq. (3.12) and (3.16) resp. (3.22c) we can now solve eq. (2.3) for the potential V finding

$$V_L^{\text{loc}}(R) = E - \frac{\hbar^2}{2M} L(L+1)/R^2 + \hbar^2/2M u_L''(R)/u_L(R) \quad (5.9)$$

Despite its simplicity eq. (5.9) might be ill-defined in the neighbourhood of zeros of u_L because of the unavoidable inaccuracies in forming the second derivative. The problems resulting from this division by zero, however, are often in such regions, where the potential is negligible anyhow. It is obvious from eq. (5.6) that V_L is energy dependent in general, since u_L depends on energy too. The second approach is based on the semiclassical WKB method. In the following we list the essential points, for details see /HO 80/. The starting point is a decomposition of the antisymmetriser A_3 , eq. (3.29), into the identity and nontrivial exchanges, which leads to direct and exchange terms /TA 81/. Rewriting eq. (5.8) in these terms yields

$$\left(-\frac{\hbar^2}{2M} \nabla^2 + V_D(R) - E\right)F(R) = - \int G(R, R') F(R') dR' \quad (5.10)$$

where G contains contributions from the kinetic energy, the interaction and the norm. Defining the Wigner transform of G by

$$G_W(R^2, p^2, (\underline{R} \cdot \underline{p})^2) = \int d\underline{s} \exp\left(\frac{i}{\hbar} \underline{s} \cdot \underline{p}\right) G(\underline{R} - \underline{s}/2, \underline{R} + \underline{s}/2) \quad (5.11)$$

we have used the symmetry and rotational invariance of G to show explicitly the functional dependence of G_W . The effective local potential V_{eff} follows from G_W via the transcendental equation /HO 80/.

$$V_{\text{eff}}(R) = G_W(R^2, 2M(E - V_{\text{eff}}(R)), 2MR^2(E - V_{\text{eff}}(R)) \frac{-\hbar^2(L+1/2)^2)}{2MR^2}) \quad (5.12)$$

Examples are numerous, for an application to the non-relativistic quark model see /FU 86/.

6. ILLUSTRATIVE EXAMPLES

In this section we try to demonstrate the flexibility of the RRGM described previously by way of example. In order to keep the presentation concise we will consider only the seven-nucleon system. We will not discuss well-known effects, like antisymmetrisation effects, or single channel results but refer mostly to recent work.

6.1 Scattering results over a wide energy range

In the ${}^7\text{Be}$ system the ${}^4\text{He} - {}^3\text{He}$ is the lowest threshold and then follows the ${}^6\text{Li} - p$ threshold. In order to explain all low-lying resonances, in addition the ${}^5\text{Li} - d$ fragmentation has to be added /H0 83, H084a/. Recently these calculation were extended /HE 87/ to include also further fragmentations like ${}^6\text{Be} + n$ to allow for a larger range of energies in cross sections and polarizations. In fig. 4 we see a typical compound nucleus behaviour at the low energy, whereas the high energy corresponds almost to diffractive scattering due to the many maxima and minima. The data of fig. 5 cover the intermediate energy range. All the gross structures are well reproduced thus demonstrating that the RRGM can reproduce complex data over a wide energy range employing one potential /ME 86/ only. More details, like polarisations and reaction cross section will be published elsewhere /HE 87/.

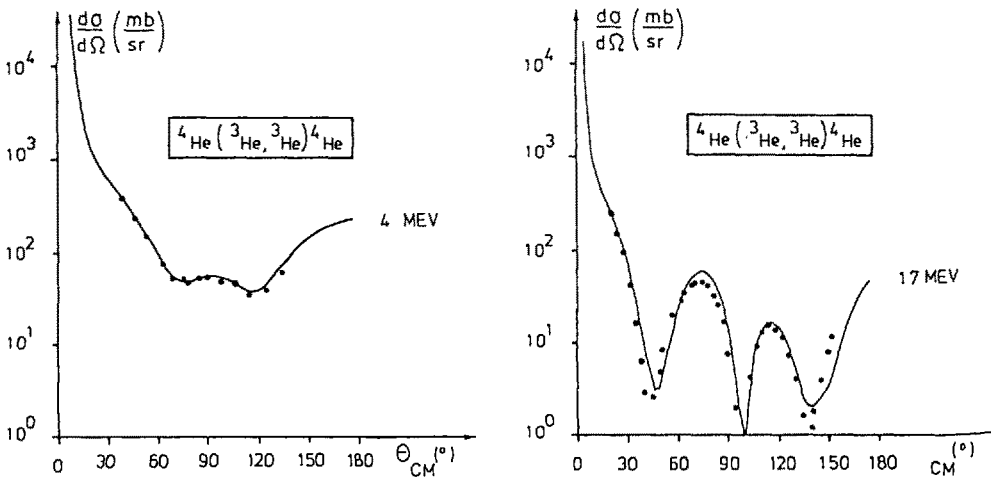


Fig. 4: Comparison of calculated ${}^3\text{He} - {}^4\text{He}$ elastic cross sections for one small and one large energy with data from /LU 78/

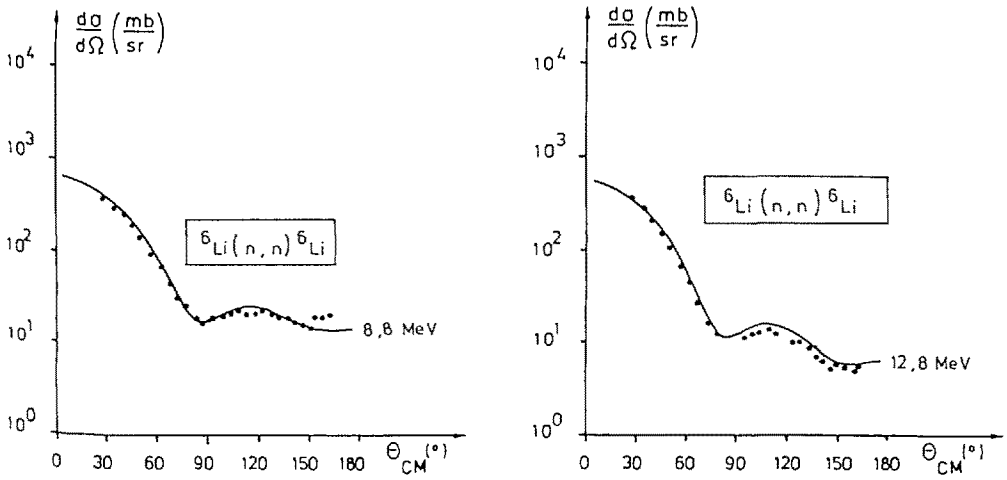


Fig. 5: Comparison of elastic neutron scattering from ${}^6\text{Li}$ for two intermediate energies with data from /H0 79/.

6.2 Expansion of the scattering wave function

In section 4 we described how to calculate ME between Gaussian functions only. From section 3, however, we know that we need ME with Coulomb functions too. As discussed in section 3 these integrals are all of short range due to the choice of kinetic energies. In fig. 6 the relative motion part of the ${}^4\text{He} - {}^3\text{He}$ wave function, eq. (3.6) is displayed, together with the expansion in terms of 15 /ST 77/ and 20 /ME 86/ Gaussian functions, where the smallest width parameters are 0.0015 fm^{-2} and 0.0001 fm^{-2} respectively.

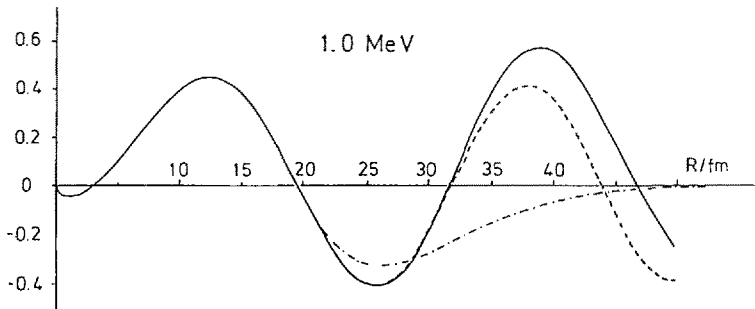


Fig. 6: Comparison of the relative motion wave function eq. (3.6) for exact Coulomb functions (full line) with expansions of the Coulomb functions into 15 Gaussians (dashed dotted line) and into 20 Gaussians (dashed line).

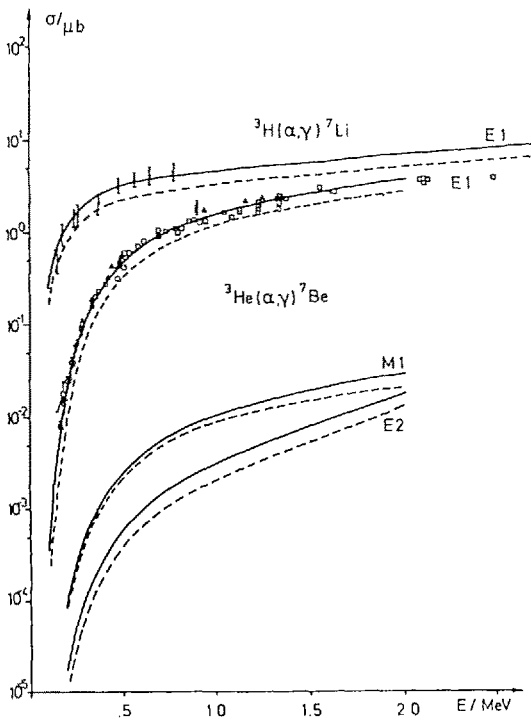


Fig. 7:

The E1-capture cross sections for the reactions ${}^3\text{He}(\alpha, \gamma){}^7\text{Be}$ and ${}^3\text{H}(\alpha, \gamma){}^7\text{Li}$ together with data. The full curves give the cross section into ground and first excited state, the dashed curves only into the groundstate. For the ${}^3\text{He}$ capture also the M1 and E2 contributions are displayed.

By way of example we see that the Gaussian expansion reproduces the correct wavefunction up to 20 and 30 fm resp. This range is even enough for electromagnetic transition operators as is shown in fig. 7, where the radiative capture cross sections ${}^4\text{He}({}^3\text{He}, \alpha){}^7\text{Be}$ and ${}^4\text{He}({}^3\text{H}, \gamma){}^7\text{Li}$ are compared to experimental data. The agreement is almost perfect, thus ruling out the ${}^4\text{He} - {}^3\text{He}$ capture reaction as source of the missing solar neutrinos. For more details see /ME 86/.

6.3 Admixtures of different fragmentations

For nuclear reactions it is well known, that different fragmentations are often the origin of resonances /HA 72/ or the occurrences of resonances in channels where they are not anticipated /HO 83, HO 84a/. We give here an example for electromagnetic transition operators, where again admixture of different fragmentations play a role.

With the existing polarised lithium ion-source sub-coulomb scattering of polarised lithium ions became feasible /EG 80/. These data allowed to determine the quadrupole moment Q and the BE2-value but also the polarisability τ simultaneously /WE 85/. The polarisability τ can be

understood as virtual excitations of the ${}^7\text{Li}$ -nucleus via E1-transitions, as indicated in fig. 8a. Whereas the BE2-value and Q are easily reproduced, poses the polarisability τ a serious problem /KA 86/.

In fig. 8b we display the integrand of the polarizability, $\tau = \int \rho dE$, as function of energy. As can be seen the integrand peaks just above the ${}^4\text{He} - {}^3\text{H}$ threshold, thus falsificating the idea of exciting the giant resonances. Besides the ${}^4\text{He} - {}^3\text{He}$ channel the ${}^6\text{Li} - n$ channel contributes another 50 percent /ME 86/, but still the calculated result is only half the experimental datum /ME 86/.

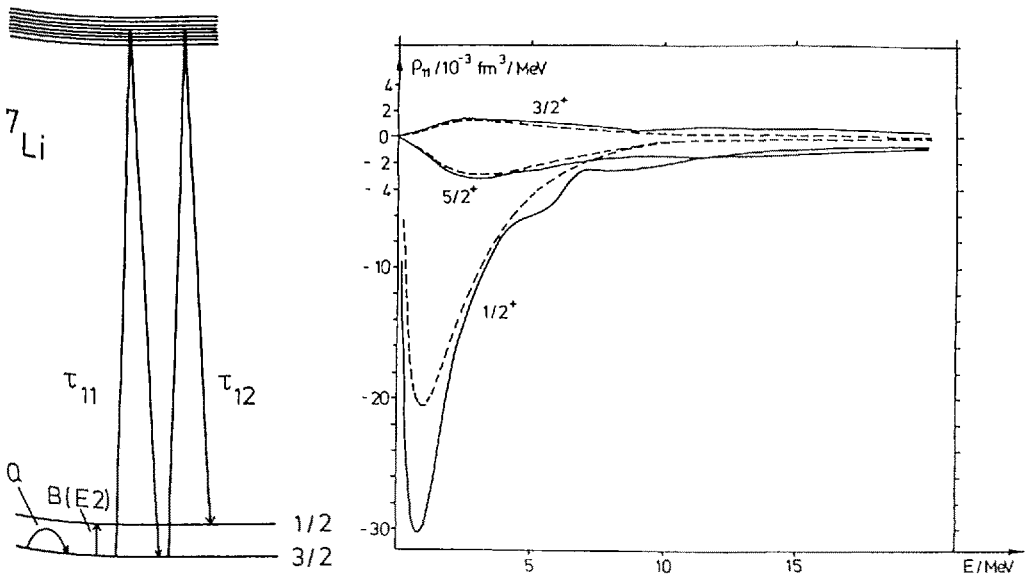


Fig. 8a: Schematic illustration of the groundstate reorientation effect (Q), the real E2-excitation (B(E2)) and the polarizability (τ_{11} and τ_{12}) via virtual E1-excitation.

b: The single partial wave contributions to the integrand ρ of the polarizability. For the dashed curves only the ${}^4\text{He} + {}^3\text{H}$ waves are taken into account, whereas the ${}^6\text{Li} + n$ channels are also considered in the full curve.

CONCLUSION

In the previous section it was shown that the microscopic RRGm method allows to describe gross structure of nuclear reactions over a wide energy range without adjustable parameters. The electromagnetic properties and the radiative capture cross sections demonstrate, that not

only the asymptotic part of the wave function, but also the wave function in the interaction region are well under control. Therefore this method should be an excellent tool to study also other properties of light nuclei, e. g. the d-state admixture in ^4He . A typical example how detailed nuclear structure information can be extracted is the tiny quadrupole moment of ^6Li /ME 84, ME 86, HO 86/. The application of the RGM to the nonrelativistic quark model allows to study the nucleon-nucleon force from a more fundamental point. Application in this direction are still numerous and very promising.

Acknowledgement

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APPENDIX A: EVALUATION OF THE COULOMB MATRIX ELEMENTS

In the following we present a derivation of the Coulomb matrix elements /BU 85, HO 84/ which relies on ideas of H. Stöwe /ST 81/. The Coulomb potential is given by

$$V_{CB} = \sum_{i < j} e_i e_j / |\underline{r}_i - \underline{r}_j| = \sum_{i < j} e_i e_j Q_{z+1}^{ij} \quad (\text{A.1})$$

where e_i is the charge of particle i and Q_{z+1}^{ij} is just the difference vector $\underline{r}_j - \underline{r}_i$. Writing $1/Q$ as

$$1/Q = 2\sqrt{\beta/\pi} \int_0^\infty dk \exp(-k^2 \beta Q^2) \quad (\text{A.2})$$

the matrix elements of the Coulomb potential are again of the form eq. (4.11) except for the additional variable Q_{z+1} and the integration over k . β is a free parameter, which is chosen appropriately later on. The integral we have to calculate now is

$$j_{CB}^{ij} L'_{\alpha'} L_{\alpha} (P_{dc}) = 2\sqrt{\beta/\pi} \int_0^\infty dk \int d\underline{s}_1 \dots d\underline{s}_{N-1} \exp(-\sum_{\mu\mu'} \rho_{\mu\mu'} \underline{s}_{\mu'} \cdot \underline{s}_{\mu} - k^2 \beta Q_{z+1}^{i'j'}) \prod_{n=1}^Z y L_n M_n(Q_n) \quad (\text{A.3})$$

The permutation P_{dc} has been applied onto the wave function to the right and onto Q_{ij} , the primes on Q_{ij} are just a reminder of that fact. Defining the generating integral analogous to eq. (4.15) and following along the lines of eqs. (4.17) to (4.20) we find

$$I_{CB}(a_1 b_1 \dots a_z b_z) = 2\sqrt{\beta/\pi} \int dk \int d_{s_1} \dots d_{s_{N-1}} \exp\left(-\sum_{\mu} \beta_{\mu} t_{\mu}^2 - k^2 \beta \sum_{\tau\tau'} P_{z+1,\tau} P_{z+1,\tau'} \underline{t}_{\tau} \cdot \underline{t}_{\tau'} + \sum_{n=1}^z a_n b_n \cdot Q_n\right) \quad (A.4)$$

With the relation $Q_{z+1} = \sum_{\tau} P_{z+1,\tau} \underline{t}_{\tau}$ being used. In order to make the evaluation of eq. (A.4) more transparent we introduce a more compact matrix notation by defining

$$\underline{t} := (\underline{t}_1, \dots, \underline{t}_{N-1})$$

$$\underline{c} := \left(\sum_{n=1}^z a_n b_n P_{n1}, \dots, \sum_{n=1}^z a_n b_n P_{n,N-1} \right) \quad (A.5)$$

and

$$B(k)_{\tau\tau'} = \beta_{\tau} (\delta_{\tau\tau'} + k^2 \beta P_{z+1,\tau} P_{z+1,\tau'} / \beta_{\tau}) =: \beta_{\tau} C_{\tau\tau'}$$

Inserting eqs. (A.5) into eq. (A.4) yields

$$\begin{aligned} I_{CB}(a_1 b_1 \dots a_z b_z) &= 2\sqrt{\beta/\pi} \int dk \int d\underline{t}_1 \dots d\underline{t}_{N-1} \exp(-\underline{t}^T B \underline{t} + \underline{c}^T \cdot \underline{t}) \\ &= 2\sqrt{\beta/\pi} \int_0^{\infty} dk \frac{\pi^{3(N-1)/2}}{(\det(B(k)))^{3/2}} \exp(\underline{c}^T B(k)^{-1} \underline{c} / 4) \end{aligned} \quad (A.6)$$

The solution is found by the methods of completing squares. We could also use this general solution in the derivation of eq. (4.21), but there the determinant and the inverse B^{-1} are trivial to calculate; therefore we renounced to introduce new quantities. For the Coulomb potential, however, this task is left to us.

Let us first consider the determinant of B . Noting that the second term of B in eq. (A.5) is a dyadic product, the determinant is given by

$$\det B = \left(\prod_{\alpha=1}^{N-1} \beta_{\alpha} \right) \left(1 + k^2 \beta \sum_{\alpha=1}^{N-1} P_{z+1,\alpha}^2 / \beta_{\alpha} \right) \quad (A.7)$$

Now we can obviously choose the free parameter β such that eq. (A.7) simplifies to

$$\det B = \left(\prod_{\alpha=1}^{N-1} \beta_{\alpha} \right) (1+k^2) \quad (\text{A.8})$$

For the evaluation of the inverse of B we again make use of the dyadic property by considering matrix C of eq. (A.5). This matrix can be written formally as

$$C = 1 + k^2 * \text{const} * \text{projector}, \quad (\text{A.9})$$

hence, the inverse of C is of the structure

$$C^{-1} = 1 + f(k) * \text{projector} \quad (\text{A.10})$$

where the function $f(k)$ is determined to

$$f(k) = -2k^2/(1+k^2) \sigma_{z+1,z+1} \quad (\text{A.11})$$

by demanding $C \cdot C^{-1} = 1$. Note that we have extended the range of indices of σ , eq. (4.23) in a natural way.

The inverse of B is now given by

$$(B^{-1})_{\alpha\alpha'} = \delta_{\alpha\alpha'} / \beta_{\alpha} - \frac{2k^2}{(1+k^2)\sigma_{z+1,z+1}} \cdot \frac{p_{z+1,\alpha}}{\beta_{\alpha}} \frac{p_{z+1,\alpha'}}{\beta_{\alpha'}} \quad (\text{A.12})$$

Inserting the determinant, eq. (A.8) and the inverse of B, eq. (A.12), into eq. (A.6) we can write the generating integral as

$$I_{CB}(a_1 b_1, \dots, a_z b_z) = 2\sqrt{2/\pi \sigma_{z+1,z+1}} \int_0^{\infty} dk \prod_{\lambda=1}^{N-1} (\pi/\beta_{\lambda})^{3/2} (1+k^2)^{-3/2} \\ \exp \left(\sum_{n>n'}^z a_n a_{n'} (b_n b_{n'} - (b_n^2 + b_{n'}^2)/2) \sigma_{nn}^{CB} \right) \quad (\text{A.13})$$

where we fixed the free parameter β as in eq. (A.8) and introduced the abbreviation

$$\sigma_{nn'}^{CB} = \sigma_{nn'} - k^2(1+k^2)^{-1} \sigma_{n,z+1} \sigma_{n',z+1} / \sigma_{z+1,z+1} \quad (\text{A.14})$$

to illustrate the correspondence between the norm integral eq. (4.21) and the Coulomb integral. This correspondence indicates how to proceed. Expanding the exponential in eq. (A.13) in powers of a_n and b_n one finds the analogous expression to eq. (4.24), except that it now contains powers of σ^{CB} . The k -integration is accomplished by expanding the powers of σ^{CB} into a binomial series.

Performing these steps the Coulomb ME are given by

$$\begin{aligned}
 r_{1m_1 \dots 1m_z}^{CB} &= 2\sqrt{2/\pi \sigma_{z+1, z+1}} \prod_{r=1}^{N-1} (\pi/B_r)^{3/2} \prod_{j=1}^z (1_j! / c_{1j m_j}) \\
 &\sum_{g_{nn'}, h_{nn'}, k_{nn'}} (-1/2)^{h_{nn'} + k_{nn'}} \prod_{n > n'} 1/(g_{nn'}, h_{nn'}, k_{nn'}) \sum_{\substack{\epsilon'_{nn'} \\ \epsilon_{nn'}}} \sigma_{nn'}^{\epsilon_{nn'}} \left(\frac{\epsilon_{nn'} + \epsilon'_{nn'}}{\epsilon_{nn'}} \right) \\
 &\left(\frac{\sigma_{n, z+1} \sigma_{n', z'+1}}{\sigma_{z+1, z+1}} \right)^{\epsilon'_{nn'}} \int_0^\infty dk (1+k^2)^{-3/2} \prod_{n > n'} \left(\frac{-k^2}{1+k^2} \right)^{\epsilon'_{nn'}} \quad (A.15)
 \end{aligned}$$

Here the $g_{nn'}$, $h_{nn'}$ and $k_{nn'}$ are determined by eqs. (4.25) and the exponents ϵ and ϵ' fulfill the relations

$$\epsilon_{nn'} + \epsilon'_{nn'} = g_{nn'} + h_{nn'} + k_{nn'}, \quad n > n' \quad (A.16)$$

The integrals over k are given in /GR 58/

$$\int_0^\infty dk (1+k^2)^{-3/2} (k^2/(1+k^2))^e = 1/(1+2e) \quad (A.17)$$

With these equations we have an exact analytic treatment of the Coulomb Potential. Combining the procedure of treating monomials in r^2 with this $1/r$ expressions, we can calculate ME of all positive powers of r . For negative powers in r additional expressions are given in /BU 85/.

APPENDIX B: THREE NUCLEON GROUND STATE WAVE FUNCTION

In order to illustrate the methods developed in the previous sections, we discuss here a simple model problem, which, however, gives already a glimpse of the ideas and techniques employed in more complicated systems. Considering the ${}^3\text{H}$ groundstate we avoid the Coulomb force and by applying the effective potential eq. (2.7) we circumvent angular momentum coupling problems.

Since this model force has no spin dependence the total spin S and total orbital angular momentum L are already good quantum numbers, hence, we need only consider states with $S = \frac{1}{2}$ and $L = 0$. The simplest wave function to comply with these requirements are the two neutrons coupled to spin zero with the additional proton leading to $S = 1/2$ and no orbital angular momentum between the nucleons. Thus we may put all three nucleons into one cluster, or the two neutrons into one cluster and the remaining proton into another one or put each nucleon into a separate cluster.

Since there is no orbital angular momentum between the two neutrons the last two fragmentations lead to identical results.

In the following we consider the fragmentation into two neutrons and the remaining proton. Let us now first consider the spin ME. The total spin function is of the form

$$|1/2 \ 1/2 \rangle = (n(+)n(-) - n(-)n(+)) \ p(+)/\sqrt{2} \quad (\text{B.1})$$

where we have explicitly given the spin projections. The spin ME eq. (4.7) for the norm and the potential is given by

$$\text{ME} = \langle 1/2 \ 1/2 || P || 1/2 \ 1/2 \rangle \quad (\text{B.2})$$

since the proton is distinguishable from the neutrons, only permutations of the two neutrons may contribute, namely $P = \text{identity}$ and $P = (12)$, the exchange of the two neutrons, hence, the only dc-symbol contributing corresponds to the identity.

The orbital ME is also easily calculated, by noting that in eq. (4.9) no spherical harmonics occur and from all permutations only the identity is left. Hence, eq. (4.11) is just a multidimensional Gaussian integral and in eq. (4.24) only the first two products differ from one. We mention in passing that for the fragmentation considered, i. e. only two orbital angular momenta, eq. (4.25) yields $k_{12} = 1$ for a relative angular momentum 1 of the proton to the first cluster.

To determine now the ground state energy, we perform the variation eq. (2.5) or (2.19). In the potential example considered in section 2.1 we found agreement between the variational approximation and the exact numerical result when using five Gaussian width parameters.

Therefore to get an idea in this three nucleon case, we again use five Gaussian width parameters for the internal function eq. (3.26), fixed to those given in table 1, and another five for the relative motion function X in eq. (3.6). If we allow all possible 25 combinations the variation yields -21.775 MeV binding energy, if we fix the internal nn-wave function to the one yielding -2.225 MeV binding, we find only -13.423 MeV in the ^3H case. We mention in passing that putting all three nucleons into one cluster only and again allowing for five free Gaussian parameters yields -21.582 MeV binding energy, just a little less than the much more complicated wave function.

From this simple example we can conclude, that in a scattering calculation the results would be bad if the internal function would be fixed to the free one. In that case additional distortion channels, where the two neutrons are in orthogonal two body states, would improve the results appreciably.

Adding a component with $l = 2$ on both relative nucleon-nucleon coordinates in a three cluster fragmentation yields another 0.4 MeV binding energy, thus demonstrating that the pure S-wave structure provides already most of the binding for such an effective force.

Contrary to that is a pure S-wave fragmentation not bounded at all for a realistic force, like /EI 71/, where the tensor potential contributes appreciably to the binding energy. In this case a two cluster configuration including a d-wave is only a poor approximation to the exact result. A three cluster configuration, however, is within 10 percent of the exact binding energy /KE 86/.

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