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A Method for the Projection of Angular Momentum

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A method is presented for the projection of a superposition of Slater determinants on states with definite angular momentum. The method can be used in the configuration mixing method or in the generator coordinate method. It is based on a projection operator of the form $e^{-i\alpha\hat{J}_z}e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}e^{-i\gamma\hat{J}_z}$, and its expectation value is expanded in powers of $e^{-i\alpha M_1}e^{-i\vartheta M_2}e^{-\vartheta M_3}$. Expectation values of operators needed for the calculation of energies and transition amplitudes between states of definite angular momenta are calculable from systems of linear equations related to these expectation values. Detailed formulas for the calculation of energy levels and transition amplitudes are presented, and algorithms suitable for computer programs are discussed.

1. INTRODUCTION

In the field of nuclear physics there exist several approximate methods for the microscopic calculation of nuclear spectra. To compare the results of calculations with experimental data, the approximate wavefunctions have to be eigenfunctions of the symmetry opeartors which commute with the Hamiltonian of the system. For example, they must have definite angular momentum quantum numbers. The angular momentum projection for the microscopic models becomes very time consuming when we are working with more than a few nucleons. For this reason, the projection of angular momentum was a subject of many publications [1]. From the computational point of view there are two suitable methods, both applicable to systems with axial symmetry. The first one [2] uses the operator $\exp(i\vartheta\hat{J}_y)$ in the projection procedure; the second one [3], the operator $\exp(\vartheta\hat{J}_-)$.

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The objective of this paper is to present a method for the exact projection of angular momentum from a linear combination of generally nonorthogonal Slater determinants. Such a function is, for example, a generator coordinate trial function [4, 5]

$$\Psi(\mathbf{r}) = \sum_k \int d\beta\, \Phi(\beta, k, \mathbf{r}) f_k(\beta), \tag{1}$$

where $\mathbf{r}$ stands for all coordinates of the n particles, β denotes a set of continuous parameters called generator coordinates, and k distinguishes different Slater determinants Φ built from different single-particle functions.

The present work generalizes the method proposed in [3] in three directions: to nonaxially symmetric systems, to calculation of transition amplitudes, and to the case when determinants $\Phi(\beta, k, \mathbf{r})$ in Eq. (1) are mutually orthogonal.

The method proposed in this paper is simpler than the method proposed by Ullah [6]. For the nonaxially symmtric basis, both methods use three independent parameters, which are related to the three Euler angles. However, in the proposed method they are real and mutually independent, which is not the case in Ullah's method.

In Sections 2 and 3 we discuss the case in which Slater determinants are eigenfunctions of the third component of angular momentum. We express the single particle functions in terms of the eigenfunctions of the harmonic oscillator in *jj* basis. For this case, a computer program already has been tested, some results of which are presented in Section 4. Also in Section 2 and 3 we treat the general case when no symmetry is imposed for Slater determinants. Discussion as to how the existing program can be extended is then presented.

2. Formulation of the Problem

There are two situations in the microscopic theory of nuclear structure in which the projection of function (1) into the subspace of definite angular momentum quantum numbers J and M is used:

(i) Projection after variation. If the amplitudes $f_k(\beta)$ of the "intrinsic" wavefunctions $\Phi(\beta, k, \mathbf{r})$ in Eq. (1) are given, we can calculate the energy levels of the projected wavefunctions $\hat{P}_M{}^J\Psi(\mathbf{r})$ as

$$E_J = \sum_{kk'} \iint d\beta\, d\beta'\, f_{k'}^*(\beta') f_k(\beta) \langle \Phi(\beta', k') | \hat{H}\hat{P}_M{}^J | \Phi(\beta, k) \rangle$$
$$\div \sum_{kk'} \iint d\beta\, d\beta'\, f_{k'}^*(\beta) f_k(\beta) \langle \Phi(\beta', k') | \hat{P}_M{}^J | \Phi(\beta, k) \rangle. \tag{2}$$

Here $\hat{P}_M{}^J$ is the projection operator projecting wavefunctions into the subspace of definite angular momentum quantum numbers J and M. The problem reduces to the evaluation of the expressions

$$\begin{aligned} &\langle \Phi(\beta', k')|\ \hat{P}_M{}^J\ |\ \Phi(\beta, k)\rangle, \\ &\langle \Phi(\beta', k')|\ \hat{H}\hat{P}_M{}^J\ |\ \Phi(\beta, k)\rangle. \end{aligned} \tag{3}$$

(ii) Projection before variation. In the generator coordinate method we usually require the energy levels (2) to be stationary with respect to the variations of the amplitudes $f_k(\beta)$. This requirement is equivalent to solving the Hill–Wheeler equations [4, 5]

$$\sum_k \int d\beta \{\langle \Phi(\beta', k')|\ \hat{H}\hat{P}_M{}^J\ |\ \Phi(\beta, k)\rangle f_k{}^J(\beta) - E^J\langle \Phi(\beta', k')|\ \hat{P}_M{}^J\ |\ \Phi(\beta, k)\rangle f_k{}^J(\beta)\} = 0. \tag{4}$$

Here we allow different amplitudes $f_k(\beta)$ for different J, so we add a superscript J: $f_k{}^J(\beta)$. Again expressions (3) appear here as the kernels of the integral equation. In the case when the dimension D_m of the space spanned by generator functions $\Phi(\beta, k, \mathbf{r})$ is finite, Eq. (4) simplifies to the equivalent form

$$\sum_k \sum_{i=1}^{D_m} \{\langle \Phi(\beta_j, k')|\ \hat{H}\hat{P}_M{}^J\ |\ \Phi(\beta_i, k)\rangle f_k{}^J(\beta_i) - E^J\langle \Phi(\beta_j, k')|\ \hat{P}_M{}^J\ |\ \Phi(\beta_i, k)\rangle f_k{}^J(\beta_i)\} = 0, \tag{5}$$

where the summation goes over D_m discrete values of coordinates β.

In order to calculate the expectation values of a tensor operator $\hat{T}_q{}^L$ (e.g., the transition amplitudes) one must also evaluate the expressions

$$\langle \Phi(\beta', k')\ |\ \hat{T}_q{}^L\hat{P}_M{}^J\ |\ \Phi(\beta, k)\rangle, \qquad q = -L, \ldots, L. \tag{6}$$

In the calculation of expressions (2) and (5), the angular momentum projection operator

$$\hat{P}_M{}^J \equiv \hat{P}^J_{MM'}\delta_{MM'} = ((2J+1)/8\pi^2)\int d\Omega\ \mathscr{D}^{*J}_{M'M}(\Omega)\ \hat{D}_R(\Omega)\ \delta_{MM'}, \tag{7}$$

is often used [2]. Here Ω stands for the three Euler angles $(\alpha, \vartheta, \gamma)$, and $\hat{D}_R(\Omega)$ is the rotation operator

$$\hat{D}_R(\Omega) = e^{-i\alpha J_z}e^{-i\vartheta J_y}e^{-i\gamma J_z} \tag{8}$$

and $\mathscr{D}^J_{M'M}(\Omega)$ is its matrix representation in the $|\, KJM\rangle$ basis:

$$\langle K'J'M' \mid \hat{D}_R(\Omega) \mid KJM\rangle = \delta_{KK'}\delta_{JJ'}\mathscr{D}_{M'M}\,. \tag{9}$$

The symbol K in $|\, KJM\rangle$ stands for all quantum numbers other than J and M.

With this projection operator, expressions (3) have the form

$$\begin{aligned}
&\langle \Phi(\beta', k')|\, \hat{P}_M{}^J \mid \Phi(\beta, k)\rangle \\
&\quad = ((2J+1)/8\pi^2) \int d\Omega\, \mathscr{D}^{*J}_{MM}(\Omega)\langle \Phi(\beta', k')|\, \hat{D}_R(\Omega) \mid \Phi(\beta, k)\rangle \\
&\text{and} \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (10)\\
&\langle \Phi(\beta', k')|\, \hat{H}\hat{P}_M{}^J \mid \Phi(\beta, k)\rangle \\
&\quad = ((2J+1)/8\pi^2) \int d\Omega\, \mathscr{D}^{*J}_{MM}(\Omega)\langle \Phi(\beta', k')|\, \hat{H}\hat{D}_R(\Omega) \mid \Phi(\beta, k)\rangle.
\end{aligned}$$

Instead of the operator $\hat{D}_R(\Omega)$ from Eq. (8), we use the operator

$$\hat{\Delta}_R(\Omega) = e^{-i\alpha\hat{J}_z}e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}e^{-i\gamma\hat{J}_z}. \tag{11}$$

A comment on differences between the operators $\hat{\Delta}_R(\Omega)$ and $\hat{D}_R(\Omega)$ is presented in Appendix 2.

The operator $\hat{\Delta}_R(\Omega)$, as well as the operator (8), has the useful property that its operation on a Slater determinant again gives a Slater determinant. Namely, using the relations

$$\hat{J}_z = \sum_{i=1}^{n} \hat{j}_{zi}\,, \qquad \hat{J}_+ = \sum_{i=1}^{n} \hat{j}_{+i}\,, \qquad \hat{J}_- = \sum_{i=1}^{n} \hat{j}_{-i}\,,$$

one gets

$$\hat{\Delta}_R(\Omega) = \prod_{i_1=1}^{n} e^{-i\alpha\hat{j}_{zi_1}} \prod_{i_2=1}^{n} e^{-\vartheta\hat{j}_{+i_2}} \prod_{i_3=1}^{n} e^{\vartheta\hat{j}_{-i_3}} \prod_{i_4=1}^{n} e^{-i\gamma\hat{j}_{zi_4}}. \tag{12}$$

The single particle operators with different particle indices commute and it follows that

$$\hat{\Delta}_R(\Omega)\,\Phi(\beta, k, \mathbf{r}) = \frac{1}{(n!)^{1/2}} \begin{vmatrix} \hat{\Delta}^1_{R_1}\varphi_1(\beta, \mathbf{x}_1) & \cdots & \hat{\Delta}^n_{R_n}\varphi_1(\beta, \mathbf{x}_n) \\ \vdots & & \vdots \\ \hat{\Delta}^1_{R_1}\varphi_n(\beta, \mathbf{x}_1) & \cdots & \hat{\Delta}^n_{R_n}\varphi_n(\beta, \mathbf{x}_n) \end{vmatrix}. \tag{13}$$

Here $\hat{\Delta}_{R_i} = e^{-i\alpha\hat{j}_{zi}}e^{-\vartheta\hat{j}_{+i}}e^{\vartheta\hat{j}_{-i}}e^{-i\gamma\hat{j}_{zi}}$ and $\varphi_i\,(\beta_1\mathbf{x}_j)$ denote the single particle functions.

Similar properties are also contained in the operator used by Ullah [6]. In the axially symmetric basis, his operator reduces to the same form as operator (11). Instead of real parameters α, ϑ, and γ as in our case, he uses complex parameters

for the nonaxially symmetric basis. These complex parameters are not linearly independent, but are related through nontrivial transcendent equations.

The operator (11) has the advantage that the expressions

$$\langle \Phi(\beta', k')| \hat{\Delta}_R(\Omega) \mid \Phi(\beta, k)\rangle, \tag{14}$$

$$\langle \Phi(\beta', k')| \hat{H}\hat{\Delta}_R(\Omega) \mid \Phi(\beta, k)\rangle, \tag{15}$$

and

$$\langle \Phi(\beta', k')| \hat{T}_q{}^L\hat{\Delta}_R(\Omega) \mid \Phi(\beta, k)\rangle \tag{16}$$

can be expressed as a set of appropriate linearly independent functions of parameters $\Omega = (\alpha, \vartheta, \gamma)$. This sum is finite if functions $\Phi(\beta, k, \mathbf{r})$ can be expressed in term of functions with finite angular momentum. As a consequence, a finite system of linear equations from expressions (14)–(16) can be obtained. This system can easily be solved. Expressions (3) and (6) can be calculated from expressions (14)–(16).

System of Equations for Matrix Elements between the Projected Functions

Axially Symmetric Basis

We shall apply the proposed projection method to the case where the basic functions $\Phi(\beta, k, \mathbf{r})$ are eigenfunctions of the operator $\hat{J}_z$. In this case the operator $\hat{\Delta}_k(\Omega)$ (Eq. (11)) simplifies (except for a trivial factor) to

$$\hat{\Delta}_R(\vartheta) = e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}. \tag{17}$$

Let us take for the single particle basis eigenfunctions of the operator $\hat{j}_{zi}$ with eigenvalues m_i. To emphasize that M_k is a good quantum number, we rewrite the basic functions in Eq. (1) in the form $\Phi(\beta, k, M_k, \mathbf{r})$. Here $M_k = \sum_{i(k)=1}^{n} m_{i(k)}$, where $i(k)$ labels the single particle functions contained in the configuration k. Let us use the trial function

$$\hat{P}_M{}^J\Psi(\mathbf{r}) = \sum_k \int d\beta\, \hat{P}^J_{MM_k}\Phi(\beta, k, M_k, \mathbf{r}) \tag{1a}$$

in order to include the basic functions with different M_k. The operators $\hat{P}^J_{MM_k}$ and $\hat{P}_M{}^J$ have the properties

$$\hat{P}^J_{MM_k} = \frac{\hat{P}_M{}^J\hat{J}_\pm^{|M-M_k|}}{B^\pm_{JM_k|M-M_k|}} = \frac{\hat{J}_\pm^{|M-M_k|}\hat{P}^J_{M_k}}{B^\pm_{JM\,|M-M_k|}},$$

$$\hat{P}^J_{MM'}\hat{P}^{J'}_{M''M''} = \hat{P}^J_{MM''}\delta_{M'M''}\delta_{JJ'},$$

$$\hat{P}_M{}^J = \hat{P}^J_{MM'}\delta_{MM'},$$

$$\hat{P}_M{}^J\hat{P}^{J'}_{M'} = \hat{P}^J_{MM'}\delta_{JJ'}\delta_{MM'}.$$

Here the + and − signs correspond to $M \geqslant M'$ and $M < M'$, respectively. The quantities B_{JMl} have the values

$$B^{+}_{JMl} = \left(\frac{(J-M)!(J+M+l)!}{(J+M)!(J-M-l)!}\right)^{1/2},$$
$$B^{-}_{JMl} = \left(\frac{(J+M)!(J-M+l)!}{(J-M)!(J+M-l)!}\right)^{1/2}. \tag{18}$$

For the trial function (1a) the secular equations

$$\sum_k \int d\beta \{\langle \Phi(\beta', k, M_{k'})| \hat{P}^J_{M_{k'},M} \hat{H} \hat{P}^J_{MM_k} | \Phi(\beta, k, M_k)\rangle$$
$$- E^J \langle \Phi(\beta', k', M_{k'})| \hat{P}^J_{M_{k'},M_k} | \Phi(\beta, k, M_k)\rangle\} f_k{}^J(\beta) = 0 \tag{4a}$$

follow. Let us introduce the notation

$$\hat{P}_M{}^J | \Phi(\beta, k, M_k)\rangle = A^J_{M_k}(\beta, k) | K, J, M\rangle \delta_{M_k M}. \tag{19}$$

From Eq. (19) it follows that

$$| \Phi(\beta, k, M_k)\rangle = \sum_{J=|M_k|}^{J_{\max}} A^J_{M_k}(\beta, k) | K, J, M_k\rangle. \tag{19a}$$

From Eqs. (19) it follows that

$$\hat{P}^J_{MM_k} | \Phi(\beta, k, M_k)\rangle = \frac{\hat{P}_M{}^J \hat{J}_{\pm}^{|M-M_k|}}{B^{\pm}_{JM_k|M-M_k|}} \sum_{J'=|M_k|}^{J_{\max}} A^{J'}_{M_k}(\beta, k) | K, J', M_k\rangle$$
$$= A^J_{M_k}(\beta, k) | K, J, M\rangle. \tag{20}$$

Let us introduce, in addition,

$$\langle \Phi(\beta', k', M_{k'})| \hat{P}^J_{M_{k'},M_k} | \Phi(\beta, k, M_k)\rangle = O^J_{M_{k'},M_k}(\beta, k, \beta', k'), \tag{21}$$

where

$$O^J_{M_{k'},M_k}(\beta, k, \beta', k') = A^{J*}_{M_{k'}}(\beta', k') A_{M_k}(\beta, k).$$

Using relation (19a), we obtain

$$e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \Phi(\beta, k, M_k)\rangle = \sum_{J=|M_k|}^{J_{\max}} A^J_{M_k}(\beta, k) \sum_{l=0}^{J+M_k} \sum_{l'=0}^{J-M_k+l}$$
$$\cdot \vartheta^{l+l'} (-1)^{l'} b^{-}_{JM_k l} b^{+}_{JM_k - ll'} | K, J, M_k - l + l'\rangle, \tag{22}$$

where

$$b^{-}_{JMl} = B^{-}_{JMl}/l! \qquad \text{and} \qquad b^{+}_{JMl} = B^{+}_{JMl}/l!.$$

The value $J_{\max}$ depends on the configuration k of the basic function $\Phi(\beta, k, M_k, \mathbf{r})$. Using Eq. (22) we obtain

$$\langle \Phi(\beta', k', M_{k'}) | e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \Phi(\beta, k, M_k) \rangle = (-1)^{M_{k'}-M_k} \vartheta^{M_{k'}-M_k} \cdot \sum_{J=|M|}^{J_{\min}} \sum_{l=m_1}^{J+M_k} (-1)^l \vartheta^{2l} b^{-}_{JM_k l} b^{+}_{JM_k - l M_{k'} - M_k + l} O^{J}_{M_{k'} M_k}(\beta, k, \beta', k'). \tag{23}$$

We have used the notation of Eq. (22) and in addition

$$\begin{aligned} M &= M_k, \qquad |M_k| \geqslant |M_{k'}|, \\ &= M_{k'}, \qquad |M_k| < |M_{k'}|, \\ J_{\min} &= \min(J_{\max}, J'_{\max}), \qquad m_1 = \max(M_k - M_{k'}, 0). \end{aligned} \tag{24}$$

The calculation of the matrix elements of Eq. (15) is quite similar. Using Eqs. (18)–(22), one obtains by means of the Wigner–Eckart theorem [7], if $\hat{H}$ is a scalar operator, the expression

$$\langle \Phi(\beta', k', M_{k'}) | \hat{H} e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \Phi(\beta, k, M_k) \rangle = (-1)^{M_{k'}-M_k} \vartheta^{M_{k'}-M_k} \cdot \sum_{J=|M|}^{J_{\min}} \sum_{l=m_1}^{J+M_k} (-1)^l \vartheta^{2l} b^{-}_{JM_k l} b^{+}_{JM_k - l M_{k'} \; M_k + l} H^{J}_{M_{k'} M_k}(\beta, k, \beta', k'), \tag{25}$$

where

$$\begin{aligned} H^{J}_{M_{k'} M_k}(\beta, k, \beta', k') &= A^{J*}_{M_{k'}}(\beta', k') \, A^{J}_{M_k}(\beta, k) \langle K' J \| \hat{H} \| K J \rangle \\ &= \langle \Phi(\beta', k', M_{k'}) | P^{J}_{M_{k'} M''} \hat{H} \hat{P}^{J}_{M' M_k} | \Phi(\beta, k, M_k) \rangle \, \delta_{M' M''} \end{aligned} \tag{26}$$

and $\langle K' J \| \hat{H} \| K J \rangle$ are reduced matrix elements. We have introduced a similar notation for overlaps $O^{J}_{M_{k'} M_k}(\beta, k, \beta', k')$ in Eq. (21). The left-hand side of Eq. (23) or Eq. (25) can be calculated as a polynomial of the parameter ϑ; let the expansion coefficients be denoted by $C^{O}_{M_{k'} M_k l}(\beta, k, \beta', k')$ and $C^{H}_{M_{k'} M_k l}(\beta, k, \beta', k')$, respectively. By comparing the coefficients at the same power of ϑ on the left and on the right-hand sides of Eq. (23) (or Eq. (25)), one obtains a triangular system of $N = J_{\min} - |M| + 1$ equations, from which expressions (21) (or (26)) can be calculated.

$$\sum_{J=|M|}^{J_{\min}} b^{-}_{JM_k} b^{+}_{JM_k - l M_{k'} - M_k + l} \begin{Bmatrix} O^{J}_{M_{k'} M_k}(\beta, k, \beta', k') \\ H^{J}_{M_{k'} M_k}(\beta, k, \beta', k') \end{Bmatrix} = \begin{Bmatrix} C^{O}_{M_{k'} M_k l}(\beta, k, \beta', k') \\ C^{H}_{M_{k'} M_k l}(\beta, k, \beta', k') \end{Bmatrix}. \tag{27}$$

The index l runs from $|M| + M_k$ to $J_{\min} + M_k$.

The formulas for the matrix elements of a tensor operator are given in Appendix 1.

The General Basis

The n particle functions in this case can be written with an additional summation over M:

$$| \Phi(\beta, k, \mathbf{r})\rangle = \sum_{J=0}^{J_{\max}} \sum_{M=-J}^{J} A^J{}_M(\beta, k) \, | K, J, M\rangle, \tag{28}$$

where $\Phi(\beta, k, \mathbf{r})$ are again Slater determinants of n single particle functions. Using Eq. (28) we obtain, with a procedure similar to that in Eq. (23), the equation

$$\begin{aligned}\langle \Phi(\beta', k')| \, e^{-i\alpha \hat{J}_z} e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} e^{-i\gamma \hat{J}_z} \, | \, \Phi(\beta, k)\rangle \\ = \sum_{J=0}^{J_{\min}} \sum_{M=-J}^{J} \sum_{l=0}^{J+M} \sum_{M'=M-l}^{J} O^J_{M'M}(\beta, k, \beta', k') \, e^{-i\alpha M'} e^{-i\gamma M} \vartheta^{2l+M'-M} \\ \cdot (-1)^{M'-M+l} b^-_{JMl} b^+_{JM-lM'-M+l} \, ,\end{aligned} \tag{29}$$

where

$$O^J_{M'M}(\beta, k, \beta', k') = \langle \Phi(\beta', k') \, | \, \hat{P}^J_{M'M} \, | \, \Phi(\beta, k)\rangle \tag{30}$$

and $J_{\min}$ is defined in Eq. (24). In the above equations we have used the notation of Eqs. (22) and (24).

To solve the system of Eqs. (29), the left-hand side has to be calculated first as a function of products $e^{-i\alpha M_1} e^{-i\gamma M_2} \vartheta^{M_3}$ for different values of the triplets (M_1, M_2, M_3). There are $N = \sum_{J=0}^{J_{\min}} (2J+1)^2$ linearly independent functions $e^{-i\alpha M_1} e^{-i\gamma M_2} \vartheta^{M_3}$. Therefore, by comparing the expansion coefficients for each function $e^{-i\alpha M_1} e^{-i\gamma M_2} \vartheta^{M_3}$ we get N linearly independent equations for the same number of unknowns $O^J_{M'M}(\beta, k, \beta', k')$. Only those quantities $O^J_{M'M}(\beta, k, \beta', k')$ which have different J and the same M and M' are couplied together. Therefore, the system of N equations splits into $(2J_{\min}+1)^2$ independent triangular systems of $J_{\min} - |M_m| + 1$ equations

$$\sum_{J=|M_m|}^{J_{\min}} O^J_{M'M}(\beta, k, \beta', k') \, b^-_{JMl} b^+_{JM-lM'-M+l} = C^O_{M'Ml}(\beta, k, \beta', k'), \tag{31}$$

where

$$l = |M_m| + M, \ldots, J_{\min} + M, \qquad \text{and} \qquad \begin{aligned} M_m &= M, & |M| &\geqslant |M'|, \\ &= M', & |M| &< |M'|. \end{aligned}$$

Each triangular system is defined by M and M' with values $-J_{\min} \leqslant M \leqslant J_{\min}$ and $-J_{\min} \leqslant M' \leqslant J_{\min}$. In Eqs. (31), $C^J_{M'Ml}$ are coefficients for the functions $e^{-i\alpha M_1} e^{-i\vartheta M_2} \vartheta^{M_3}$ on the left-hand side of Eq. (29).

The calculation of $H^J_{M'M}(\beta, k, \beta', k')$ is similar to the calculation of $O^J_{M'M}(\beta, k, \beta', k')$.

3. An Example of the Calculation of the Coefficients $C^O_{M'Ml}(\beta, k, \beta', k')$ and $C^H_{M'Ml}(\beta, k, \beta', k')$

We shall discuss here a rather standard case in nuclear physics when it is convenient to express the single particle basis $\varphi_i(\beta, \mathbf{x}_j)$ (Sect. 2, Eq. (13)), in terms of functions ($|\mu\rangle \equiv |n_\mu l_\mu j_\mu m_{i_\mu}\rangle$) in jj basis [7],

$$|\varphi_i(\beta, \mathbf{x}_j)\rangle = \sum_\mu C_{i\mu}(\beta)\,|\mu\rangle. \tag{32}$$

Here l_μ is orbital angular momentum, j_μ is total angular momentum, m_{j_μ} is its third projection, and n_μ stands for all other quantum numbers.

Let us first calculate expression (14). Taking into account Eq. (13), we have

$$\langle\Phi(\beta', k')|\,\hat{\Delta}_R(\Omega)\,|\,\Phi(\beta, k)\rangle = \det(N(\beta, k, \beta', k')), \tag{33}$$

where

$$\begin{aligned} N_{ij}(\beta, k, \beta', k') &\equiv \langle\varphi_i(\beta')|\,\hat{\Delta}_R(\Omega)\,|\,\varphi_j(\beta)\rangle \\ &= \sum_{\mu\nu} C_{i\mu}(\beta')\,C_{j\nu}(\beta)\langle\mu\,|\,\hat{\Delta}_R\,|\,\nu\rangle. \end{aligned} \tag{34}$$

Let the Hamiltonian of the system be as usual a scalar operator of the form

$$\hat{H} = \sum_i \hat{T}(\mathbf{x}_i) + \sum_{i<j} \hat{V}(\mathbf{x}_i, \mathbf{x}_j). \tag{35}$$

The matrix elements (15) can be written [8]

$$\begin{aligned} \langle\Phi(\beta', k')|\,\hat{H}\hat{\Delta}_R(\Omega)\,|\,\Phi(\beta, k)\rangle &= \sum_{\mu\nu} T_{\mu\nu} R(\mu\hat{\Delta}_R\nu) \\ &\quad + (1/2!) \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} R(\mu\nu\hat{\Delta}_R\rho\hat{\Delta}_R\sigma). \end{aligned} \tag{36}$$

Here,

$$R(\mu\hat{\Delta}_R\nu) = \sum_\mu \sum_{ij} C^*_{i\mu}(\beta')\,C_{j\mu'}(\beta)\langle\nu\,|\,\hat{\Delta}_R\,|\,\mu'\rangle\,\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k') \tag{37}$$

and

$$\begin{aligned} R(\mu\nu\hat{\Delta}_R\rho\hat{\Delta}_R\sigma) = \sum_{\rho'\sigma'} \sum_{ijlm} & C^*_{i\mu}(\beta')\,C^*_{j\nu}(\beta')\,C_{l\rho'}(\beta)\,C_{m\sigma'}(\beta) \\ & \cdot \langle\rho\,|\,\hat{\Delta}_R\,|\,\rho'\rangle\langle\sigma\,|\,\hat{\Delta}_R\,|\,\sigma'\rangle\,\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k'), \end{aligned} \tag{38}$$

where $\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k')$ and $\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k')$ are the first and the second order minors of the matrix $N(\beta, k, \beta', k')$. Here $T_{\mu\nu}$ and $V_{\mu\nu\rho\delta}$ are expectation values of the one-body operator $\hat{T}(\mathbf{x}_1)$ and the two-body operator $\hat{V}(\mathbf{x}_1, \mathbf{x}_2)$, respectively, in the basis $|\mu\rangle$. Eq. (36) is discussed in more detail in Appendix 3.

In the case when $\det(N(\beta, k, \beta', k'))$, Eq. (33), does not vanish, the matrix $N(\beta, k, \beta', k')$ can be inverted and its minors $\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k')$ and $\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k')$ in Eqs. (37) and (38) can be expressed by elements of the inverse of $N(\beta, k, \beta', k')$ [8]:

$$M(\beta, k, \beta', k') = ((N(\beta, k, \beta', k'))^T)^{-1}. \tag{39}$$

Then $\langle \Phi(\beta', k')| \hat{H}\hat{\Delta}_R(\Omega) | \Phi(\beta, k)\rangle$ can be written in a form which is much more convenient for calculation, since one can work with inverse matrices which have smaller dimensions than the minors in Eq. (36).

$$\begin{aligned}\langle \Phi(\beta', k')| \hat{H}\hat{\Delta}_R(\Omega) | \Phi(\beta, k)\rangle &= \sum_{\mu\nu} T_{\mu\nu}\mathscr{P}_{\mu\nu}(\beta, k, \beta', k') \\ &+ \tfrac{1}{2}\sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma}[\mathscr{P}_{\mu\rho}(\beta, k, \beta', k')\,\mathscr{P}_{\nu\sigma}(\beta, k, \beta', k') - \mathscr{P}_{\mu\sigma}(\beta, k, \beta', k') \\ &\cdot \mathscr{P}_{\nu\rho}(\beta, k, \beta', k')]/\det(N(\beta, k, \beta', k')).\end{aligned} \tag{40}$$

The meaning of the new symbol $\mathscr{P}$ is

$$\begin{aligned}\mathscr{P}_{\mu\nu}(\beta, k, \beta', k') = \sum_{\mu'}\sum_{ij} C^*_{i\mu}(\beta')\, C_{j\mu'}(\beta)\, M_{ij}(\beta, k, \beta', k') \\ \cdot \det(N(\beta, k, \beta', k'))\langle \nu | \hat{\Delta}_R | \mu'\rangle.\end{aligned} \tag{41}$$

In Appendix 3, formula (40) is expressed in more detail for the case when single particle states are eigenstates of the isospin operator.

When the configurations k and k' are not the same, then $\det(N(\beta, k, \beta', k')) = 0$. Since it is easier numerically to work with matrices of a smaller number of dimensions, in Appendix 4 we have derived an algorithm which enables us to write an equation similar to Eq. (40) also in this case.

3.1. *Axially Symmetric Basis*

In this case the operator $\hat{\Delta}_k(\Omega)$ has a simple form (Eq. (17)) and Eq. (32) simplifies in the sense that the summation goes only over those single particle functions having the same value of the third projection of the total angular momentum. The single particle overlaps $\langle \mu | \hat{\Delta}_k(\Omega) | \nu\rangle$ in Eq. (34) are polynomials in ϑ of the order $2j_\nu + m_{j_\mu} - m_{j_\nu}$:

$$\begin{aligned}\langle \mu | e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \nu\rangle = \sum_{l=m_0}^{j_\nu+m_{j_\nu}} \vartheta^{2l+m_{j_\mu}-m_{j_\nu}} b^+_{j_\nu m_{j_\nu} - l m_{j_\mu} - m_{j_\nu} + l} \\ \cdot (-1)^{m_{j_\mu}-m_{j_\nu}+l} b^-_{j_\nu m_{j_\nu} l}\, \delta_{n_\mu n_\nu}\delta_{l_\mu l_\nu}\delta_{j_\mu j_\nu},\end{aligned} \tag{42}$$

where $m_0 = \max(m_{j_\nu} - m_{j_\mu}, 0)$.

In order to determine the coefficients $O^J_{M'M}(\beta, k, \beta', k')$ and $H^J_{M'M}(\beta, k, \beta', k')$ in Eq. (27) (or (31)), we have to express the scalar products (33) and matrix elements of the Hamiltonian (36) or (40) in the form

$$\langle \Phi(\beta', k', M') | e^{-\vartheta J_+} e^{\vartheta J_-} | \Phi(\beta, k, M) \rangle = (-1)^{M'-M} \vartheta^{M'-M} \sum_{l=0}^{N} C^O_{M'Ml}(\beta, k, \beta', k')\, \vartheta^{2l} (-1)^l$$

and (43)

$$\langle \Phi(\beta', k', M') | \hat{H} e^{-\vartheta J_+} e^{\vartheta J_-} | \Phi(\beta, k, M) \rangle = (-1)^{M'-M} \vartheta^{M'-M} \sum_{l=0}^{N} C^H_{M'Ml}(\beta, k, \beta', k')\, \vartheta^{2l} (-1)^l,$$

where $N = J_{\min} - M + 1$. The coefficients $C^O_{M'Ml}(\beta, k, \beta', k')$ and $C^H_{M'Ml}(\beta, k, \beta', k')$ can be calculated by computer using polynomial algebra.

3.2. *General Basis*

In this case the summation in Eq. (32) generally goes over all μ, and the operator $\Delta_k(\Omega)$ from Eq. (11) must be used in Eqs. (33) and (36):

$$\langle \mu | e^{-i\alpha J_z} e^{-\vartheta J_+} e^{\vartheta J_-} e^{-i\gamma J_z} | \nu \rangle = e^{-i\alpha m_{j_\mu}} e^{-i\gamma m_{j_\nu}} \sum_{l=m_0}^{j_\mu + m_{j_\nu}} \vartheta^{2l + m_{j_\mu} - m_{j_\nu}} \cdot (-1)^{m_{j_\mu} - m_{j_\nu} + l} b^+_{j_\nu m_{j_\nu} - l m_{j_\mu} - m_{j_\nu}} b^-_{j_\nu m_{j_\nu} l} \delta_{n_\mu n_\nu} \delta_{l_\mu l_\nu} \delta_{j_\mu j_\nu}, \tag{44}$$

m_0 being already defined in Eq. (42).

Again, in order to identify the coefficients $O^J_{M'M}(\beta, k, \beta', k')$ in Eq. (29) and coefficients $H^J_{M'M}(\beta, k, \beta', k')$ from the corresponding equations, we write scalar products (33) and the corresponding matrix elements in the form

$$\langle \Phi(\beta', k') | e^{-i\alpha J_z} e^{-\vartheta J_+} e^{\vartheta J_-} e^{-i\gamma J_z} | \Phi(\beta, k) \rangle = \sum_{M, M' = -J_{\min}}^{J_{\min}} \sum_{l=0}^{N} C^O_{M'Ml}(\beta, k, \beta', k')\, e^{-i\alpha M'} e^{-i\gamma M} \vartheta^{2l + M' - M} (-1)^{M'-M+l} \tag{45}$$

and similarly

$$\langle \Phi(\beta', k') | \hat{H} e^{i\alpha J_z} e^{-\vartheta J_+} e^{\vartheta J_-} e^{-i\gamma J_z} | \Phi(\beta, k) \rangle = \sum_{M, M' = -J_{\min}}^{J_{\min}} \sum_{l=0}^{N} C^H_{M'Ml}(\beta, k, \beta', k')\, e^{-i\alpha M'} e^{-i\gamma M} \vartheta^{2l + M' - M} (-1)^{M'-M+l} \tag{46}$$

with $J_{\min}$ defined in Eq. (24) and N in Eq. (43). The calculation of the coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$ is similar to that in the case of an axially symmetric basis. The difference is that we must now work with linearly independent functions of the form $e^{-i\alpha M_1} e^{-i\gamma M_3} \vartheta^{M_2}$ instead of with polynomials alone.

4. Numerical Calculations

The method described has been applied in nuclear structure to calculate the low-lying excited states of light nuclei and transition rates between the states [5a, 11]. For all cases chosen we have used the axially symmetric basis and the program has also been written only for these cases.

4.1. *Discussion of the Program*

We discuss here the case when the overlap matrix $N(\beta, k, \beta', k')$ is not singular and therefore Eq. (40) can be used.

As can be seen from Sections 2 and 3, the main part of the numerical work in the projection procedure reduces to the calculation of the coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$, (Eq. (27)). The most time-consuming part of this calculation is to find the elements of the inverse of matrix $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$, (Eq. (39), (41)), as polynomials of the parameter ϑ. This can be done in two alternative ways:

(i) The first possibility is to work entirely with polynomial algebra. This means that all transformations needed to find the coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$ are done in such a way that the parameter ϑ is treated as a formal parameter and that one works with coefficients for different powers of ϑ only. The advantage of this procedure is a good numerical accuracy. By using a symbolic algebra with integers, the accuracy can even be improved. The disadvantage is that the matrix $\mathscr{P}(\beta, k, \beta', k')$ is stored as a three-dimensional array, since one dimension is used for the coefficients of polynomials $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$. Therefore, quite a large computer memory is needed. The dimension of the matrices reduces by a factor of 2, due to the fact that polynomials are either even or odd.

(ii) Another possibility is to work entirely with numbers: to calculate the values of expressions (33) and (40) for m discrete values of parameter ϑ and at the end to calculate back from these values the coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$.

As the orthogonality[1] of the two functions ϑ^l and $\vartheta^{l'}$ is rather bad for large

[1] The scalar product is defined by $\int_{-\pi}^{\pi} \vartheta^l \vartheta^{l'} \sin \vartheta \, d\vartheta$.

l and l', it is better to use more orthogonal functions. One can introduce [3] $\vartheta = e^{i\varphi}$ and calculate expressions (33) and (40) for $2m + 1$ values of ϑ

$$\vartheta_j = e^{i\varphi_j} = e^{i(2\pi j/(2m+1))} = \cos\varphi_j + i\sin\varphi_j\,, \tag{47}$$

where $m \geqslant \mathcal{M}$, if $\mathcal{M}$ is the maximal power of ϑ in expression (33) or (40). At the end, the coefficients $C^O_{M'Ml}(\beta, k, \beta', k')$, $C^H_{M'Ml}(\beta, k, \beta', k')$ can be calculated by Fourier analysis. In this case the elements $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$ are numbers and the matrix is only two-dimensional. The program is simpler since no polynomial algebra is needed. Nevertheless, all the expressions have to be calculated at $2\mathcal{M} + 1$ points.

In our program we compromise between these two possibilities. We work with polynomial algebra everywhere except when calculating the inverse of the matrix $N(\beta, k, \beta', k')$, where we use the second procedure. (The reason is that in this case a standard program for matrix inversion can also be used.) This combination of two procedures introduces a limitation on the accuracy of calculations. One must be very cautious when dividing the products of inverse matrices $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$ in Eq. (40) by $\det(N(\beta, k, \beta', k'))$. The polynomials are divisible in principle, but the round-off might cause trouble. One proposal for avoiding such trouble is discussed in Appendix 5. In all the calculations we have done using this proposal remainders never exceeded the value 10^{-6}. (See also Section 4.2, where an estimate of the overall error is given.)

Once the coefficients $C^O_{M'Ml}(\beta, k, \beta', k')$ and $C^H_{M'Ml}(\beta, k, \beta', k')$ are calculated, the triangular systems of Eqs. (27) can easily be solved. As a result we get the expressions $\langle\Phi(\beta', k', M')|\,\hat{P}^J_{M'M}\,|\,\Phi(\beta, k, M)\rangle$ (Eq. (21)), and $\langle\Phi(\beta', k', M')|\,\hat{P}^J_{M'M''}\hat{H}\hat{P}^J_{M''M}\,|\,\Phi(\beta, k, M)\rangle$ (Eq. (26)), which are needed in the secular equation

$$\mathscr{H}^J_{M'M}X^J - E^J\mathscr{O}^J_{M'M}X^J = 0, \tag{48}$$

must be solved for each $J = \max(|\,M'\,|, |\,M\,|),\ldots, J_{\min}$. Here $\mathscr{H}^J_{M'M}$ and $\mathscr{O}^J_{M'M}$ are matrices, the dimension of which depends on the choice of the number of configurations k and of the discrete values of the set of parameters β, and the X^J are corresponding eigenvectors.

Once the polynomials $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$ (Eq. (41)) are calculated, expectation values of any transition operator (Eq. (6)) can also be obtained. The derivation of the corresponding formulas is shown in Appendix 1.

The extension of the existing program to the general case is formally quite straightforward. From the formulas in Section 2 it can be seen that the matrix $\mathscr{P}_{\mu\nu}(\beta, k, \beta', k')$ now must be five-dimensional, the last three dimensions being reserved for the coefficients for different triples (M_1, M_2, M_3) (see Section 2).

The coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$ are now the coefficients for the functions $e^{-i\alpha M_1}e^{-i\gamma M_2}\vartheta^{M_3}$. From experience with the axially symmetric case, it is difficult to estimate the numerical errors for the general case if approach (ii) with Fourier analysis is used. If it turns our that approach (ii) is not accurate enough, approach (i) with polynomial algebra or symbolic algebra must be developed.

4.2. *Application of the Method. The Low-Lying States of the* ^{20}Ne *Nucleus*

As an illustration, we shall show here the results of a calculation of the low-lying states of even parity of the ^{20}Ne nucleus calculated with the generator coordinate method [5a].

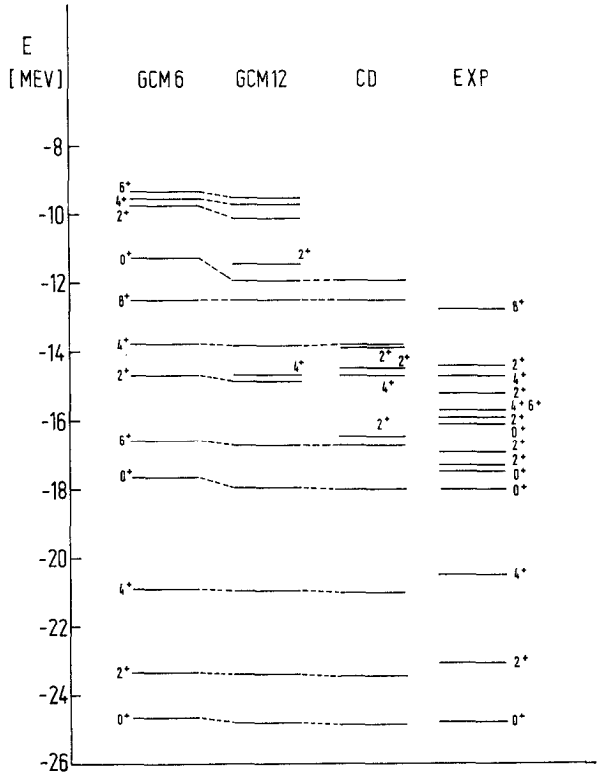

FIG. 1. The low-lying states of even parity of the ^{20}Ne nucleus are calculated with the generator coordinate method with one configuration k and six (GCM6) and twelve (GCM12) discrete values for the pair of generator coordinates β and μ, respectively (Eq. (49)). The method proposed in this paper for the projection into the subspace of definite angular momentum is used. For illustration, the experimental data (EXP) and the results of the complete diagonalization (CD) method [12], calculated for the same single particle model space as in the generator coordinate calculations, are added.

We have used a model in which the two protons and two neutrons outside the closed shell of ^{16}O determine the properties of the system. They interact with the Kuo effective interaction ($\hat{H}_{eff} = \hat{U} + \hat{V}_{eff}$) [9], which is calculated for the model space of all Slater determinants from the single particle eigenfunctions of the harmonic oscilator operator in the $1d$–$2s$ shell. Here $\hat{U}$ is a one-body operator with the expectation values $\langle 1d\frac{5}{2}m_j \mid \hat{U} \mid 1d\frac{5}{2}m_j\rangle = 0.00$ MeV, $\langle 1d\frac{3}{2}m_j \mid \hat{U} \mid 1d\frac{3}{2}m_j\rangle = 5.08$ MeV and $\langle 2s\frac{1}{2}m_j \mid U \mid 2s\frac{1}{2}m_j\rangle = 0.87$ MeV. For the single particle functions $\mid nljm_j\rangle$ the notation from Section 3 is used. The effective interaction $\hat{V}_{eff}$ is calculated for the model space of the functions of the $1d$–$2s$ shell.

For the single particle functions $\varphi_j(\beta, \mathbf{x}_j)$ in Eq. (32), we have chosen the eigenfunctions of Nilsson's axially symmetric potential [10]:

$$\hat{h} = \hbar\omega_0\tfrac{1}{2}(-\nabla^2 + r^2) + \hbar\omega_0\beta r^2 y_{20} + C\mathbf{ls} + \mu l^2, \tag{49}$$

choosing β and μ as the two generator coordinates. We have taken that configuration k_0 which corresponds to the lowest sum of the single particle energies, and six and twelve discrete values for the two generator coordinates β and μ, respectively. Following the procedure described for the angular momentum projection, we calculated expressions (21) and (26) and then solved the eigenvalue problem (48).

One result of the calculations is shown in Fig. 1. The calculation has been done on a CDC 6400 computer (in single precision arithmetic.) The projection procedure is estimated to be accurate to at least six decimal places. We estimated this accuracy from a comparison with the results obtained with a program based on a different [11] projection method.

The proposed projection method has already been applied to different nuclear systems, and the results of some of the calculations have been published [5a, 11].

APPENDIX 1: MATRIX ELEMENTS OF TENSOR OPERATORS

Let $\hat{T}_q^L$ be any tensor operator of order L. Let $\Psi^u_{J_uM_u}$ be wavefunctions of the states between which the matrix elements of the tensor operator have to be calculated. If these states are solutions of Eq. (5), one obtains by using Eqs. (19) and (20)

$$\langle \Psi^u_{J_uM_u} \mid \hat{T}_q^L \mid \Psi^v_{J_vM_v}\rangle = \sum_{kk'}\sum_{ij} f^{J_u}_{k'}(\beta_j)\langle \Phi(\beta_j, k')\, \hat{P}^{J_u}_{M_u} \mid \hat{T}_q^L \mid \hat{P}^{J_v}_{M_v}\Phi(\beta_i, k)\, f^{J_v}_k(\beta_i)$$

$$= \sum_{kk'}\sum_{ij} f^{J_u}_{k'}(\beta_j)\, A^{J_u*}_{M_u}(\beta_j, k')\, A^{J_v}_{M_v}(\beta_i, k)\, f^{J_v}_k(\beta_i)\langle K'J_uM_u \mid \hat{T}_q^L \mid KJ_vM_v\rangle. \tag{1.1}$$

Using the Wigner–Eckart theorem [7], one can write

$$\langle \Psi^u_{J_u M_u} \| \hat{T}_q{}^L \| \Psi^v_{J_v M_v} \rangle = \sum_{kk'} \sum_{ij} f^{J_u}_{k'}(\beta_j)(T^L)^{J_u J_v}_{M_u M_v}(\beta_i, k, \beta_j, k') f^{J_v}_k(\beta_i), \quad (1.2)$$

where

$$(T^L)^{J_u J_v}_{M_u M_v}(\beta_i, k, \beta_j, k') = A^{J_v}_{M_v}(\beta_i, k) A^{J_u *}_{M_u}(\beta_j, k') \langle K' J_u M_u \| \hat{T}_q{}^L \| K J_v M_v \rangle$$

$$= \langle \Phi(\beta_j, k') \hat{P}^{J_u}_{M_u} \| \hat{T}_q{}^L \| \hat{P}^{J_v}_{M_v} \Phi(\beta_i, k) \rangle. \quad (1.3)$$

The expressions $\langle \Psi^u_{J_u M_u} \| \hat{T}_q{}^L \| \Psi^v_{J_v M_v} \rangle$, $\langle K' J_u M_u \| \hat{T}_q{}^L \| K J_v M_v \rangle$, and $\langle \Phi(\beta_j, k') \hat{P}^{J_u}_{M_u} \| \hat{T}_q{}^L \| \hat{P}^{J_v}_{M_v} \Phi(\beta_i, k) \rangle$ are the corresponding reduced matrix elements [7], independent of q, M_u, and M_v. Expressions (1.3) can be calculated using the proposed projection method in the following way.

(a) If the basic functions $\Phi(\beta_i, k, \mathbf{r})$ (Eq. (1)), have axial symmetry, then Expressions (1)–(3) can be calculated using operator (17) and Eqs. (22) and (1.2):

$$\langle \Phi(\beta_j, k', M_{k'}) | \hat{T}_q{}^L e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \Phi(\beta_i, k, M_k) \rangle$$

$$= \sum_{J=|M_k|}^{J_{\max}} \sum_{J'=|M_{k'}|}^{J'_{\max}} A^{J'*}_{M_{k'}}(\beta_j, k') A^{J}_{M_k}(\beta_i, k) \langle K' J' M_{k'} | \hat{T}_q{}^L e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | K J M_k \rangle$$

$$= \sum_{J=|M_k|}^{J_{\max}} \sum_{J'=|M_{k'}|}^{J'_{\max}} \sum_{l=0}^{J+M_k} \sum_{l'=0}^{J-M_k+l} \vartheta^{l+l'}(-1)^{l'} b^-_{JM_k l} b^+_{JM_k - l l'}(-1)^{2L}$$

$$\cdot \langle J' M_{k'} | J L M_k - l + l' q \rangle (T^L)^{J' J}_{M_{k'} M_k}(\beta_j, k', \beta_i, k). \quad (1.4)$$

The symbols $\langle J' M_{k'} | J L_{M_k} q \rangle$ are Clebsch–Gordan coefficients [7]. Equation (1.4) can be written in a more compact way as

$$\langle \Phi(\beta_j, k', M_{k'}) | \hat{T}_q{}^L e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} | \Phi(\beta_i, k, M_k) \rangle = \sum_{J=|M_k|}^{J_{\max}} \sum_{J'=F_1(J)}^{F_2(J)} \sum_{l=m_1}^{m_2}$$

$$\cdot (-1)^{2L} \vartheta^{2l+M_m}(-1)^{l+M_m} b^-_{JM_k l} b^+_{JM_k - l M_m + l} \langle J' M_{k'} | J L M_{k'} - q q \rangle$$

$$\cdot (T^L)^{J' J}_{M_{k'} M_k}(\beta_i, k, \beta_j, k'), \quad (1.5)$$

where the meanings of the symbols are

$$\begin{aligned} M_m &= -q + M_{k'} - M_k\,, \\ F_1(J) &= \max(|\,J - L\,|, |\,M_{k'}\,|), \\ F_2(J) &= \min(J + L, J'_{\max}), \\ m_1 &= \max(q + M_k - M_{k'}\,, 0), \\ m_2 &= J + q, \end{aligned} \tag{1.6}$$

and b^{-}_{JMl} is defined in Eq. (22).

To determine the unknowns $(T^L)^{J'J}_{M_{k'}M_k}(\beta_i\,, k, \beta_j\,, k')$, the left-hand side of Eq. (1.5) must first be calculated. If $\hat{T}_q{}^L$ is a one-body operator, one obtains from Eq. (40) the expression

$$\langle \Phi(\beta_j\,, k', M_{k'})|\ \hat{T}_q{}^L e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-}\ |\ \Phi(\beta_i\,, k, M_k)\rangle = \sum_{\mu\nu} \langle \mu\ |\ \hat{T}_q{}^L\ |\ \nu\rangle\, \mathscr{P}_{\mu\nu}(\beta_i\,, k, \beta_j\,, k'). \tag{1.7}$$

The quantity $\mathscr{P}_{\mu\nu}(\beta_i\,, k, \beta_j\,, k')$ is defined in Eq. (41), and $\langle \mu\ |\ \hat{T}_q{}^L\ |\ \nu\rangle$ are matrix elements between single particle spherical functions defined in Section 3.

The quantities $\mathscr{P}_{\mu\nu}(\beta_i\,, k, \beta_j\,, k')$ are polynomials of parameter ϑ. As we can see from Eq. (1.5), the polynomials are either odd if M_m is odd, or even if M_m is even. By comparing the coefficients for different powers of ϑ on the left-hand and right-hand sides of Eq. (1.5), one gets a system of equations for each $q = -L$, $-L + 1$,..., L from which the unknowns $(T^L)^{J'J}_{M_{k'}M_k}(\beta_i\,, k, \beta_j\,, k')$ can be calculated. Once the expressions $(T^L)^{J'J}_{M_{k'}M_k}(\beta_i\,, k, \beta_j\,, k')$ are known, Eq. (1.2) can be solved.

(b) For a nonaxial symmetric basis, the operator $\hat{\Delta}_k(\Omega)$ from Eq. (11) must be used. Then the following expression must be evaluated.

$$\begin{aligned} \langle \Phi(\beta_j\,, k')|\ \hat{T}_q{}^L e^{-i\alpha \hat{J}_z} e^{-\vartheta \hat{J}_+} e^{\vartheta \hat{J}_-} e^{-i\gamma \hat{J}_z}\ |\ \Phi(\beta_i\,, k)\rangle = \sum_{J=0}^{J_{\max}} \sum_{J'=|J-L|}^{F_2(J)} \sum_{M_k=-J}^{J} \\ \cdot \sum_{M_{k'}=-J'}^{J'} \sum_{l=m_1}^{m_2} (-1)^{2L+l+M_m} e^{-i\alpha M_{k'}} e^{-i\gamma M_k} b^{-}_{JM_kl} \vartheta^{2l+M_m} \\ \cdot\, b^{+}_{JM_k-lM_m+l} (T^L)^{J'J}_{M_{k'}M_k}(\beta_i\,, k, \beta_j\,, k') \langle J'M_{k'}\ |\ JLM_k{}' - qq\rangle. \end{aligned} \tag{1.8}$$

The notation of Eq. (1.6) has been used.

The left-hand side of Eq. (1.8) has a structure similar to that in case (a), if $\hat{T}_q{}^L$ is again a one-body operator. The elements $\mathscr{P}_{\mu\nu}(\beta_i\,, k, \beta_j\,, k')$ are now expressed

as coefficients of linearly independent functions $e^{-i\alpha M_{k'}}e^{-i\gamma M_k}\vartheta^{2l+M_m}$. Therefore the sum can be expressed in the same form. By equalizing the coefficients of different functions on the left- and right-hand sides of Eq. (1.8), one obtains the systems of equations for the unknowns $(T^L)^{J'J}_{M_{k'}M_k}(\beta_i, k, \beta_j, k')$.

APPENDIX 2: COMPARISON OF THE OPERATORS $\hat{D}_R(\Omega)$ AND $\hat{\Delta}_R(\Omega)$

It is shown in Section 2 that by using the operator $\hat{\Delta}_R(\Omega)$ one can in general obtain a system of equations for unknowns $\langle\Phi(\beta', k')|\ \hat{P}_{M'}{}^{J}\ |\ \Phi(\beta, k)\rangle$. The system of equations splits into independent systems, coupling together equations for quantities $\langle\Phi(\beta', k')|\ \hat{P}_{M'}{}^{J}\ |\ \Phi(\beta, k)\rangle$ which have the same M and different J. This splitting is caused by the two factors $e^{-i\alpha\hat{J}_z}$ and $e^{-i\gamma\hat{J}_z}$ of the operator $\hat{\Delta}_R(\Omega)$ (Eq. (29)). The remaining part of the operator $\hat{\Delta}_R(\Omega)$, the factor $e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}$, generally plays a similar role as when applied in the case of an axially symmetric basis. Since the two operators, $\hat{\Delta}_R(\Omega)$ and $\hat{D}_R(\Omega)$, differ only in the factor depending on ϑ, it is enough to discuss the case when the basis is axially symmetric.

In the axially symmetric case (Section 2), the operator $\hat{\Delta}_k(\Omega)$ reduces to

$$\hat{\Delta}_R(\Omega) = e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}, \tag{2.1}$$

while the operator $\hat{D}_k(\Omega)$ is

$$\hat{D}_R(\Omega) = e^{-i\vartheta\hat{J}_y} = e^{-(\vartheta/2)(\hat{J}_+-\hat{J}_-)}. \tag{2.2}$$

One can express the expectation value of the operator (2.1) between two Slater determinants,

$$\langle\Phi(\beta', k', M_{k'})|\ e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}\ |\ \Phi(\beta, k, M_k)\rangle, \tag{2.3}$$

as a power series in the parameter ϑ with coefficients which contain the unknowns $\langle\Phi(\beta', k', M_{k'})|\ \hat{P}^{J}_{M_{k'}M_k}\ |\ \Phi(\beta, k, M_k)\rangle$ (Eq. (43)). If the Slater determinants $\Phi(\beta, k, M_k)$ have a nonzero projection into the finite subspace of the functions with definite angular momentum quantum numbers, the power of the polynomial is of finite degree.

This is not the case if the operator (2.2) is used:

$$\langle\Phi(\beta', k', M_{k'})|\ e^{-(\vartheta/2)(\hat{J}_+-\hat{J}_-)}\ |\ \Phi(\beta, k, M_k)\rangle. \tag{2.4}$$

One has

$$e^{-(\vartheta/2)(\hat{J}_+-\hat{J}_-)}\ |\ \Phi(\beta, k, M_k)\rangle = \sum_{J=|M_k|}^{J_{\max}} A^{J}_{M_k}(\beta, k) \sum_{l=0}^{\infty} (-\vartheta/2)^l \frac{1}{l!} (\hat{J}_+ - \hat{J}_-)^l\ |\ KJM_k\rangle$$

$$= \sum_{J=|M_k|}^{J_{\max}} A^{J}_{M_k}(\beta, k) \sum_{l=0}^{\infty} (-\vartheta/2)^l \frac{1}{l!} \sum_i \sum_{\text{perm}} (-1)^i (J_+)^{l-i}(J_-)^i\ |\ KJM_k\rangle. \tag{2.5}$$

By multiplying the left-hand side of Eq. (2.5) by $\langle\Phi(\beta', k', M_{k'})|$ one gets a system of an infinite numbers of equations, except in the trivial case when $J_{\max} = 0$. Only N of these equations are linearly independent, with $N = \text{minimum}(J_{\max}, J'_{\max}) - \text{maximum}(|M_{k'}|, |M_k|) + 1$. The symbol $\sum_{\text{perm}}$ means the summation over all possible combinations in which the operator $\hat{J}_+$ has the power $(l - i)$ and the operator $\hat{J}_-$ the power i. The other symbols are defined in Section 2.

The operator $e^{-\vartheta\hat{J}_+}e^{\vartheta\hat{J}_-}$ has another advantage which is important in our projection procedure; when applying it to a Slater determinant, it transforms each single particle function (Eq. (13)) to a finite sum of functions multiplied by different powers of ϑ. Therefore the elements of the overlap matrix (Eq. (33)) are polynomials of a finite power in ϑ. In the case of the operator $e^{-(\vartheta/2)(\hat{J}_+ - \hat{J}_-)}$ these sums are power series with infinite power of ϑ. The evaluation of the determinant of the overlap matrix as a polynomial of ϑ is therefore much less straightforward.

APPENDIX 3: CALCULATION OF THE EXPECTATION VALUES OF THE HAMILTON OPERATOR

Let the Hamiltonian of the system be of form (35). By using Eq. (13) we can write [8] the expectation values of the operator $\hat{H}\hat{\Delta}_R(\Omega)$ between Slater determinants $\Phi(\beta, k, \mathbf{r})$ in the form

$$\langle\Phi(\beta', k')|\,\hat{H}\hat{\Delta}_R(\Omega)\,|\,\Phi(\beta, k)\rangle = \sum_{ij}\langle\varphi_i(\beta')|\,\hat{T}\,|\,\hat{\Delta}_R(\Omega)\varphi_j(\beta)\rangle \cdot \mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k') + (1/2!)\sum_{ijlm}\langle\varphi_i(\beta')\,\varphi_j(\beta')|\,\hat{V}\,|\hat{\Delta}_R(\Omega)\varphi_l(\beta)\,\hat{\Delta}_R(\Omega)\varphi_m(\beta)\rangle \cdot \mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k'). \tag{3.1}$$

The notation is the same as in Section 3. If we express the functions $\varphi_i(\beta, \mathbf{x}_j)$ in the way used in Eq. (32), and if we insert the completeness relation

$$\sum_{\mu'}|\,\mu'\rangle\langle\mu'\,| = 1 \tag{3.2}$$

to the left of the operator $\hat{\Delta}_R(\Omega)$, whenever it appears on the right-hand side of Eq. (3.1), we get Eq. (36) (Section 3). The transformation from Eq. (3.1) to Eq. (36) is exact even in a truncated single particle basis, if all spherical single particle functions with the same n_μ, l_μ, j_μ and all different m_{j_μ} are included. Namely, the expressions $\langle\mu\,|\,\hat{\Delta}_R\,|\,\nu\rangle$, (Eq. (37)) which follow when using Eq. (3.2), are different from zero only if $n_\mu = n_\nu$, $l_\mu = l_\nu$, $j_\mu = j_\nu$.

Usually the single particle basis $\varphi_i(\beta, \mathbf{x}_j)$ have definite isospin quantum numbers [5a]. In this case the matrix $N(\beta, k, \beta', k')$ from Eq. (34) has the form

$$N(\beta, k, \beta', k') = \begin{bmatrix} N^{(p)}(\beta, k, \beta', k') & 0 \\ 0 & N^{(n)}(\beta, k, \beta', k') \end{bmatrix}, \tag{3.3}$$

where the indices p and n denote the proton and the neutron overlap matrices. Then the scalar product of Eq. (33) from Section 3 can be rewritten as

$$\begin{aligned} \langle \Phi(\beta', k') | \hat{\Delta}_R(\Omega) | \Phi(\beta, k) \rangle &= \det(N^{(p)}(\beta, k, \beta', k') \det(N^{(n)}(\beta, k, \beta', k')) \\ &= D^{(p)}(\beta, k, \beta', k') D^{(n)}(\beta, k, \beta', k'). \end{aligned} \tag{3.4}$$

Similarly the expectation value of the Hamiltonian $\hat{H}$ (Eq. (40), Section 3) can be written in a more convenient form for calculation as

$$\begin{aligned} \langle \Phi(\beta', k') | \hat{H}\hat{\Delta}_R(\Omega) | \Phi(\beta, k) \rangle &= \sum_{\mu\nu} T_{\mu\nu} (\mathscr{P}^{(p)}_{\mu\nu}(\beta, k, \beta', k') D^{(n)}(\beta, k, \beta', k') \\ &+ \mathscr{P}^{(n)}_{\mu\nu}(\beta, k, \beta', k') D^{(p)}(\beta, k, \beta', k')) + (1/2) \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma} [\{\mathscr{P}^{(p)}_{\mu\rho}(\beta, k, \beta', k') \\ &\cdot \mathscr{P}^{(p)}_{\nu\sigma}(\beta, k, \beta', k') - \mathscr{P}^{(p)}_{\mu\sigma}(\beta, k, \beta', k') \mathscr{P}^{(p)}_{\nu\rho}(\beta, k, \beta', k')\} \\ &\cdot D^{(n)}(\beta, k, \beta', k')/D^{(p)}(\beta, k, \beta', k') \\ &+ \{\mathscr{P}^{(n)}_{\mu\rho}(\beta, k, \beta', k') \mathscr{P}^{(n)}_{\nu\sigma}(\beta, k, \beta', k') - \mathscr{P}^{(n)}_{\mu\sigma}(\beta, k, \beta', k') \mathscr{P}^{(n)}_{\nu\rho}(\beta, k, \beta', k')\} \\ &\cdot D^{(p)}(\beta, k, \beta', k')/D^{(n)}(\beta, k, \beta', k') + \mathscr{P}^{(p)}_{\mu\rho}(\beta, k, \beta', k') \mathscr{P}^{(n)}_{\nu\sigma}(\beta, k, \beta', k') \\ &+ \mathscr{P}^{(p)}_{\nu\sigma}(\beta, k, \beta', k') \mathscr{P}^{(n)}_{\mu\rho}(\beta, k, \beta', k')], \end{aligned} \tag{3.5}$$

where

$$\mathscr{P}^{(p)}_{\mu\nu} = \sum_{\mu'} \sum_{i,j \in p} C^*_{i\mu}(\beta') C_{j\mu'}(\beta) M_{ij}(\beta, k, \beta', k') D^{(p)}(\beta, k, \beta', k') \langle \nu | \hat{\Delta}_R | \mu' \rangle.$$

The summation goes only over those i and j which determine proton states. The expression for $\mathscr{P}^{(n)}_{\mu\nu}$ follows by replacing index p by n.

APPENDIX 4: The Calculation of the Expectation Values of Operators if the Determinant of the Overlap Matrix is Zero

We have expressed the expectation value of the Hamilton operator either with minors of the overlap matrix (Eq. (36)) or with elements of the inverse transpose matrix (Eq. (40)) to the overlap matrix (Eq. (34)) if its determinant is nonzero.

For numerical calculations with a computer it is more convenient to work with elements of the inverse matrix, to reduce storage requirements. The number of second order minors which appear in Eq. (40) is equal to r^4, while the number of elements of the corresponding inverse matrix is equal to r^2, where r is the rank of the overlap matrix.

The determinant of the overlap matrix $N(\beta, k, \beta', k')$ is equal to zero whenever any one of the transformed single particle functions from the right-hand-side Slater determinant $\hat{\Delta}_R(\Omega)\varphi_i(\beta, \mathbf{x}_j)$ (Eq. (33)) is orthogonal to all the single particle functions $\varphi_i(\beta, \mathbf{x}_j)$ from the left-hand-side Slater determinant, or vice versa. In this case the inverse to the matrix $N(\beta, k, \beta', k')$ does not exist. However, Eq. (40) can still be used in a slightly modified form. We shall show this in the following example.

Let us assume that the τth single particle function $\varphi_\tau(\beta', \mathbf{x}_j)$ is orthogonal to all transformed functions:

$$\langle \varphi_\tau(\beta') | \hat{\Delta}_R(\Omega) | \varphi_i(\beta) \rangle = 0, \tag{4.1}$$

where index i runs over all the single particle functions of the right-hand-side Slater determinant. Then only those minors of the first rank $\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k')$ in Eq. (3.1) will be nonzero which have index i equal to τ, and only those minors of the second rank $\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k')$ (Eq. (3.1)) are different from zero which have either index i or index j equal to τ. Then the formula (3.1) can be written as

$$\begin{aligned}\langle \Phi(\beta', k') | \hat{H}\hat{\Delta}_R(\Omega) | \Phi(\beta, k) \rangle = \sum_{ij} \langle \varphi_i(\beta') | \hat{T} | \hat{\Delta}_R \hat{\Delta}_R(\Omega)\varphi_j(\beta) \rangle \mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k') \\ \cdot \delta_{i\tau} + (1/2!) \sum_{ijlm} \langle \varphi_i(\beta')\, \varphi_j(\beta') | \hat{V} | \hat{\Delta}_R(\Omega)\varphi_l(\beta)\, \hat{\Delta}_R(\Omega)\varphi_m(\beta) \rangle \mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k') \\ \cdot (\delta_{i\tau} + \delta_{j\tau})(1/(1 + \delta_{ij})).\end{aligned} \tag{4.2}$$

We shall make use of the property of minors that the two minors $\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k')$ and $\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k')$ of the overlap matrix $N(\beta, k, \beta', k')$ are independent of the value of the element $N_{ij}(\beta, k, \beta', k')$. Let us put the element $N_{\tau\tau}(\beta, k, \beta', k')$ of the overlap matrix equal to 1 and let us denote $\tilde{N}(\beta, k, \beta', k')$ this new overlap matrix. Let us denote the corresponding minors as $\tilde{\mathscr{R}}^{(1)}_{ij}(\beta, k, \beta', k')$ and $\tilde{\mathscr{R}}^{(2)}_{ijlm}(\beta, k, \beta', k')$. Then we can write

$$\begin{aligned}&\mathscr{R}^{(1)}_{ij}(\beta, k, \beta', k') = \tilde{\mathscr{R}}^{(1)}_{ij}(\beta, k, \beta', k') \qquad \text{if} \quad i = \tau \\ &\text{and} \\ &\mathscr{R}^{(2)}_{ijlm}(\beta, k, \beta', k') = \tilde{\mathscr{R}}^{(2)}_{ijlm}(\beta, k, \beta', k') \qquad \text{if} \quad i = \tau \quad \text{or} \quad j = \tau.\end{aligned} \tag{4.3}$$

Since

$$\tilde{\mathscr{R}}^{(1)}_{ij} = \det(\tilde{N}(\beta, k, \beta', k'))\, \tilde{M}_{ij}(\beta, k, \beta', k')$$

and

$$\tilde{\mathscr{R}}^{(2)}_{ijlm} = = \det(\tilde{N}(\beta, k, \beta', k'))\tilde{M}(_{il}(\beta, k, \beta', k')\, \tilde{M}_{jm}(\beta, k, \beta', k') - \tilde{M}_{im}(\beta, k, \beta', k')\, \tilde{M}_{jl}(\beta, k, \beta', k')), \tag{4.4}$$

where $\tilde{M}(\beta, k, \beta', k')$ is the inverse transposed matrix to the matrix $\tilde{N}(\beta, k, \beta', k')$, Eq. (4.2) can be rewritten in the form

$$\langle \Phi(\beta', k')|\, \hat{H}\hat{\Delta}_R(\Omega)\, |\, \Phi(\beta, k)\rangle = \det(\tilde{N}(\beta, k, \beta', k') \sum_{ij} \langle \varphi_i(\beta')|\, \hat{T}\, |\, \hat{\Delta}_R\hat{\Delta}_R(\Omega)\varphi_j(\beta)\rangle$$

$$\cdot\, \tilde{M}_{ij}(\beta, k, \beta', k')\, \delta_{i\tau} + (1/2!)\det(\tilde{N}(\beta, k, \beta', k')$$

$$\cdot \sum_{ijlm} \langle \varphi_i(\beta')\, \varphi_j(\beta')|\, \hat{V}\, |\, \hat{\Delta}_R(\Omega)\varphi_l(\beta)\, \hat{\Delta}_R(\Omega)\varphi_m(\beta)\rangle$$

$$\cdot\, (\tilde{M}_{il}(\beta, k, \beta', k')\, \tilde{M}_{jm}(\beta, k, \beta', k')(\delta_{i\tau} + \delta_{j\tau})(1/(1 + \delta_{ij}))$$

$$- \tilde{M}_{im}(\beta. k, \beta', k')\, \tilde{M}_{jl}(\beta, k, \beta', k')(\delta_{i\tau} + \tau_{j\tau})(1/(1 + \delta_{ij}))). \tag{4.5}$$

If, as in Eq. (41), we introduce

$$\tilde{\mathscr{P}}_{\mu\nu}(\beta, k, \beta', k') = \sum_{\mu'} \sum_{ij} C^*_{i\mu}(\beta')\, C_{j\mu'}(\beta)\, \tilde{M}_{ij}(\beta, k, \beta', k')\, \det(\tilde{N}(\beta, k, \beta', k'))$$

$$\cdot \langle \nu |\, \hat{\Delta}_R\, |\, \mu'\rangle\, \delta_{i\tau}\,,$$

there follows an equation similar to Eq. (40):

$$\langle \Phi(\beta', k')|\, \hat{H}\hat{\Delta}_R(\Omega)\, |\, \Phi(\beta, k)\rangle = \sum_{\mu\nu} T_{\mu\nu}\tilde{\mathscr{P}}_{\mu\nu}(\beta, k, \beta', k') + (1/2!)$$

$$\cdot \sum_{\mu\nu\rho\sigma} V_{\mu\nu\rho\sigma}[\tilde{\mathscr{P}}_{\mu\rho}(\beta, k, \beta', k')\, \tilde{\mathscr{P}}_{\nu\sigma}(\beta, k, \beta', k') - \tilde{\mathscr{P}}_{\mu\sigma}(\beta, k, \beta', k')\, \tilde{\mathscr{P}}_{\nu\rho}(\beta, k, \beta', k')]$$

$$\cdot\, (1/\det(\tilde{N}(\beta, k, \beta', k'))). \tag{4.6}$$

In a similar way formulas can be derived for the case when one of the transformed single particle functions $\hat{\Delta}_R(\Omega)\varphi_i(\beta, \mathbf{x}_j)$ from the right-hand-side Slater determinant $\hat{\Delta}_R(\Omega)\Phi(\beta, k, \mathbf{r})$ is orthogonal to all single particle functions $\varphi_j(\beta', \mathbf{x}_k)$ from the left-hand-side Slater determinant, or if two transformed single particle functions from the left- (from the right)-hand-side Slater determinants are orthogonal to all (transformed) single particle functions from the right- (from the left)-hand-side Slater determinant. In the last case, the expectation values of the one-body operator $\hat{T}(\mathbf{x}_i)$ are equal to zero and only the two-body operator $\hat{V}(\mathbf{x}_i, \mathbf{x}_j)$ gives nonzero

contributions, since a one-body operator can change only one particle state at the same time.

If more than two (transformed) single particle functions from the left (from the right)-hand side Slater determinant are orthogonal to all others from the right- (from the left)-hand-side Slater determinant, then the expectation value of the two-particle operator $\hat{V}(\mathbf{x}_i, \mathbf{x}_j)$ is also equal to zero.

APPENDIX 5: A USEFUL EXPERIENCE WITH THE DIVISION OF POLYNOMIALS

The polynomials which appear as divisors and dividends in expressions for the expectation values of the Hamilton operator (Eqs. (40), (3.5)) are in principle divisible without remainders. Since we work with real algebra, it can happen that even small numerical errors ($<10^{-5}$) in divisors and dividends cause the remainders after division to be by no means negligible. This does not happen if one works either entirely with polynomial algebra with integer coefficients, or with numbers and finds the coefficients $C^{O}_{M'Ml}(\beta, k, \beta', k')$ and $C^{H}_{M'Ml}(\beta, k, \beta', k')$ by Fourier analysis at the very end. Using the combined approach, the following algorithm is proposed to avoid trouble with round-offs.

Let a polynomial $C(\vartheta)$ (with coefficient c_i, $i = 1,..., n_c$) be divided by a polynomial $A(\vartheta)$ (with coefficients a_i, $i = 1,..., n_a$), to obtain a polynomial $B(\vartheta)$ (with coefficients b_i, $i = 1,..., n_b$). The symbols n_a, n_b, and n_c are coefficients at maximal powers of the corresponding polynomials. The following relation is valid: $n_b = n_c - n_a$, if $C(\vartheta)$ is even and $A(\vartheta)$ is odd, and $n_b = n_c - n_a + 1$, in all other cases.

The coefficients of the polynomial $B(\vartheta)$ can be expressed with recursive formulas in two ways: either by starting with coefficients at the highest power of the polynomials $C(\vartheta)$ and $A(\vartheta)$,

$$b_{n_b-i+1} = (1/a_{n_a})(c_{n_c-i+1} - \delta \sum_{l=0}^{i-2} b_{n_b-l} a_{n_a-i+l+1}), \qquad i = 1,..., n_b,$$
$$\delta = 0, \quad \text{if} \quad i-2 < 0, \qquad \delta = 1, \quad \text{otherwise}, \tag{5.1}$$

or by starting with coefficients at the lowest power of the polynomials,

$$b_{i-k+1} = (1/a_k)(c_{i+i_d} - \sum_{l=1}^{\min(i-k, n_a-k)} a_{k+l} b_{i-k-l+1}), \tag{5.2}$$

$i = k,..., n_b + k - 1$, if k is the first nonzero coefficient at the lowest power of the polynomial $A(\vartheta)$ and $i_d = 1$, if $C(\vartheta)$ is even and $A(\vartheta)$ is odd; and $i_d = 0$, otherwise.

The inaccuracy of the calculated coefficients goes up with increasing index i in both formulas (5.1) and (5.2). From this it follows that the smallest round-off errors appear if the coefficients at the lowest powers of the polynomial $B(\vartheta)$ are calculated by means of formula (5.2), and those of the highest by means of formula (5.1). Experience has shown that in all the cases treated, the numerical errors are such that in the projection procedure the errors produced are no larger than 10^{-6}.

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