АКАДЕМИЯ НАУК УКРАИНСКОЙ ССР

ИНСТИТУТ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

ITP-86-25E

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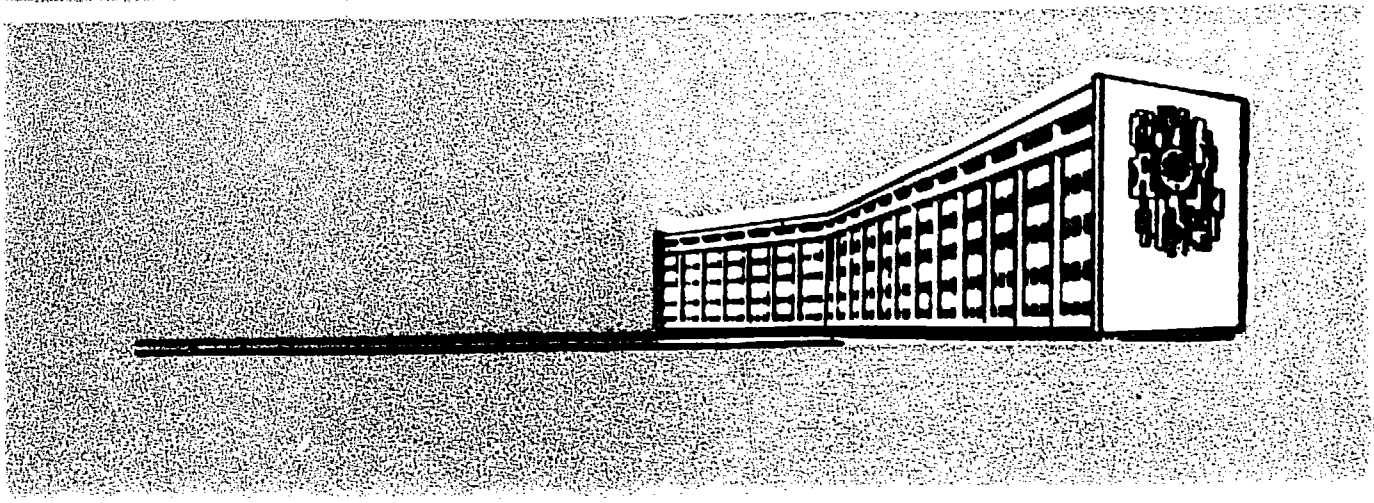
GENERATING MATRIX ELEMENTS OF THE HAMILTONIAN OF THE ALGEBRAIC VERSION OF RESONATING GROUP METHOD ON INTRINSIC WAVE FUNCTIONS WITH VARIOUS OSCILLATOR LENGTHS



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Preprint
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Kiev - 1986

УДК 539.143.3; 539.144.3

Бадалов С.А., Филиппов Г.Ф.

Производящие матричные элементы гамильтониана алгебраической версии метода резонирующих групп на внутренних волновых функциях с различными осцилляторными длинами

Даны рецепты вычисления производящих матричных элементов алгебраической версии метода резонирующих групп (МРГ) для двух- и трехкластерных систем нуклонов, причем движение центра масс выделяется точно. Для гамильтониана с гауссовской зависимостью нуклон-нуклонного потенциала производящие матричные элементы алгебраической версии МРГ можно записать явно, если известны матричные элементы соответствующей системы на волновых функциях кластерной модели Бринка.

Badalov S.A., Filippov G.F.

Generating Matrix Elements of the Hamiltonian of the Algebraic Version of Resonating Group Method on Intrinsic Wave Functions with Various Oscillator Lengths

The receipts to calculate the generating matrix elements of the algebraic version of resonating group method (RGM) are given for two- and three-cluster nucleon systems, the center of mass motion being separated exactly. For the Hamiltonian with Gaussian nucleon-nucleon potential dependence the generating matrix elements of the RGM algebraic version can be written down explicitly if matrix elements of the corresponding system on wave functions of the Brinc cluster model are known.

INTRODUCTION

The resonating group method (RGM) is now the basic microscopic approach used to describe the continuous spectrum states of interacting nuclei [1]. The algebraic version of RGM formulated in Refs. [2-5], in contrast to a traditional formalism, is reduced to solving not the integodifferential equations but a system of homogeneous algebraic equations

$$\sum_{m} \langle n|\hat{H}|m\rangle C_m - E\dot{C}_n = 0. \qquad (1)$$

Besides the algebraic version is attractive due to simplicity of the algorithm of calculating the matrix elements between basis functions with arbitrarily given excitation quanta values and also due to the possibility to employ the known asymptotic behaviour C_n at large n [3].

The solution of Eq. (1) gives the wave functions of a relative motion of subsystems which allows one to calculate readily the photoproduction and γ capture reactions and the probabilities of radiation transitions [5].

The algebraic version of RGM proved to be capable to solve the problem of describing the collective resonances in a system of nucleons excited under the light atomic nuclei scattering by means of both the cluster basis and the collective modes of multinucleon system's excitation [6,7].

At the same time within the RGM algebraic version there has not yet been formulated the algorithm for calculating the generating matrix elements of the Hamiltonian for the case when intrinsic wave functions of interacting nuclei have different oscillator lengths. This has essentially restricted the possibilities for the intrinsic wave functions variation according to the given nucleon-nucleon potentials and has not admitted a sufficiently correct reproduction of thresholds of the different channels.

Our paper gives the algorithm for calculating the generating matrix elements of the RGM algebraic version with no identity of oscillator lengths being assumed.

Interacting nuclei may have wave functions with different oscillator lengths. The center-of-mass motion is separated exactly owing to an employment of the double Fourier-transformation

method proposed in Ref.[8]. The receipts to calculate the RGM generating matrix lements in oscillator representation are deduced both for two- and three-cluster systems with different oscillator lengths.

Realization of the algorithm suggested makes it possible to describe correctly both the structure and the dynamics of interacting nuclei, to trace the changes in their polarization in a process of collision.

1. DEFINITION OF CENTER OF MASS MOTION

It has been shown by Tohsaki-Suzuki [8] how one can obtain the RGM matrix elements from the matrix elements of operators on cluster wave functions of the Brinc model with different oscillator lengths.

The wave function of two-cluster Brink model has the form

$$|\Psi(S)\rangle = \hat{A} \exp\left[-\frac{1}{a_1^2}\sum_{i=1}^{A_1}(\vec{r}_i-\vec{S}_1)^2\right] \exp\left[-\frac{1}{a_2^2}\sum_{i=A_1+1}^{A_1+A_2}(\vec{r}_i-\vec{S}_2)^2\right] \chi_1 \chi_2 , \qquad (2)$$

where $\vec{S}_1$ and $\vec{S}_2$ are radii of the vector of oscillator fields centers, a_1 and a_2 are oscillator radii of the fields of first and second clusters. $\hat{A}$ is antisymmetrization operator. It is assumed that there are no more than four nucleons in every cluster ($A_i \leq 4$).

To ensure translational invariance we superpose the reference frame with the oscillator field centre

$$\sum_i A_i \vec{S}_i = 0 . \qquad (3)$$

Let now turn from one-particle coordinates to the Jacobi ones following the formulas

$$\sum_{i=1}^{A_2} r_i^2 = \sum_{i=1}^{A_2-1} q_i^2 + A_2 R_{10}^2 , \qquad A_2 \vec{R}_{10} = \sum_{i=1}^{A_2} \vec{r}_i ,$$

$$\sum_{i=A_1+1}^{A_1+A_2} r_i^2 = \sum_{i=A_1}^{A_1+A_2-2} q_i^2 + A_2 R_{20}^2 , \qquad A_2 \vec{R}_{20} = \sum_{i=A_1+1}^{A_1+A_2} \vec{r}_i , \qquad (4)$$

$$A_1 \vec{R}_{10} + A_2 \vec{R}_{20} = A \vec{R}_0 , \qquad \vec{q}_1 = \sqrt{\frac{A_1 A_2}{A_1+A_2}} \left(\vec{R}_{20} - \vec{R}_{10}\right) ,$$

where $\vec{q}_0$ is the Jacobi coordinate of a relative mo ion of clusters, $\vec{R}_0$ is the coordinate of centre-of-mass of nucleons system. Then the wave function (2) can be written as follows

$$|\Psi(S)\rangle = \hat{A}\,\Phi_1\,\Phi_2\,\exp\left[-\alpha R_0^2 + \beta\vec{R}_0\left(\vec{q}_0-\vec{S}\right) - \frac{1}{2}\gamma\left(\vec{q}_0-\vec{S}\right)^2\right], \quad (5)$$

where Φ_1 and Φ_2 are intrinsic wave functions of clusters, $\vec{S}$ is the Jacobi generator coordinate of a relative distance between oscillator fields centres of clusters

$$\vec{S} = \sqrt{\frac{A_1A_2}{A_1+A_2}}\left(\vec{S}_2-\vec{S}_1\right) \quad (6)$$

In (5) the following notations are introduced

$$\alpha = \frac{1}{2}\left(\frac{A_1}{a_1^2}+\frac{A_2}{a_2^2}\right), \qquad \beta = \sqrt{\frac{A_1A_2}{A_1+A_2}}\left(\frac{1}{a_1^2}-\frac{1}{a_2^2}\right),$$
$$\gamma = \frac{1}{A_1+A_2}\left(\frac{A_2}{a_1^2}+\frac{A_1}{a_2^2}\right) \quad (7)$$

Since the oscillator radii in various clusters are different (see (5)) the exponent has the term proporional to ($\vec{R}_0\vec{q}_0$). That's why we cannot exclude the centre-of-mass motion multiplier. It was noticed by Tohsaki-Suzuki (8) the Fourier transformation from the space of generator coordinates $\vec{S}$ to the space of momenta $\vec{K}$ permits to split the vectors $\vec{R}_0$ and $\vec{q}_0$. Then after separation of the centre-of-mass motion multiplier and carrying out the Fourier transformation from the momenta space $\vec{K}$ to the space of parameteric coordinates of the relative motion of clusters $\vec{q}$ we get the RGM traditional matrix element [1]

$$\left\langle \delta\left(\vec{\tilde{q}}-\vec{q}_0\right)\tilde{\Phi}_1\tilde{\Phi}_2\left|\hat{H}\hat{A}\right|\Phi_1\Phi_2\,\delta\left(\vec{q}-\vec{q}_0\right)\right\rangle =$$

$$= \frac{\left(\gamma\tilde{\gamma}\omega\right)^{3/2}}{(2\pi)^9}\int\cdots\int d\vec{R}\,d\vec{S}\,d\vec{\tilde{R}}\,d\vec{\tilde{S}}\,\langle\tilde{\Psi}(R)|\hat{H}|\Psi(S)\rangle \times \quad (8)$$

$$\times\exp\left[i\vec{\tilde{K}}\left(\vec{\tilde{q}}-\vec{R}\right)-i\vec{K}\left(\vec{q}-\vec{S}\right)+\frac{1}{4\omega}\left(\frac{\beta\vec{K}}{\gamma}-\frac{\tilde{\beta}\vec{\tilde{K}}}{\tilde{\gamma}}\right)^2+\frac{K^2}{2\gamma}+\frac{\tilde{K}^2}{2\tilde{\gamma}}\right],$$

where

$$\omega = \alpha + \tilde{\alpha} - \frac{\beta^2}{2\gamma} - \frac{\tilde{\beta}^2}{2\tilde{\gamma}}$$

The RGM matrix element is to the left in (8) and to the right there is multiple integral from multiparticle matrix element of translationally invariant operator $\hat{H}$ on functions (2) of the cluster Brinc model with various oscillator radii $\langle \tilde{\Psi}(R)|\hat{H}|\Psi(S)\rangle$. The latter is calculated traditionally by integrating over all one-particle variables. $\vec{R}$ is the Jacobi coordinate of a relative distance between oscillator fields centres of the function "bra". Parameters $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\gamma}$ are expressed through the nucleon numbers B_1 and B_2 , and oscillator radii b_1 and b_2 in clusters of "bra" functions by formulas (7) after transformation $A_i \to B_i$ and $a_i \to b_i$.

For three-cluster systems the RGM matrix element is expressed via the multiparticle matrix element of the three-cluster Brinc model with various oscillator radii in the following way

$$\langle \delta(\vec{\tilde{q}}_1 - \vec{\tilde{a}}_{10})\,\delta(\vec{\tilde{q}}_2 - \vec{\tilde{a}}_{20})\,\tilde{\Phi}_1\tilde{\Phi}_2\tilde{\Phi}_3\,|\hat{H}\hat{A}|\,\Phi_1\Phi_2\Phi_3\,\delta(\vec{q}_1 - \vec{a}_{10})\,\delta(\vec{q}_2 - \vec{a}_{20})\rangle =$$

$$= \left(\Gamma\tilde{\Gamma}Q\right)^{3/2} \int\cdots\int d\vec{K}_1\, d\vec{K}_2\, d\vec{\tilde{K}}_1\, d\vec{\tilde{K}}_2\, d\vec{Q}_1\, d\vec{Q}_2\, d\vec{P}_1\, d\vec{P}_2\, \langle \tilde{\Psi}(R)|\hat{H}|\Psi(S)\rangle \times \qquad (9)$$

$$\times \exp\left\{ \frac{1}{2\Gamma}\left(\gamma_2 K_1^2 + \gamma_1 K_2^2 - 2\alpha\beta_1 \vec{K}_1\vec{K}_2\right) + \frac{1}{2\tilde{\Gamma}}\left(\tilde{\gamma}_2 \tilde{K}_1^2 + \tilde{\gamma}_1 \tilde{K}_2^2 - 2\tilde{\alpha}\tilde{\beta}_1 \vec{\tilde{K}}_1\vec{\tilde{K}}_2\right) + \right.$$

$$+ \frac{1}{4Q}\left[\frac{\vec{K}_1\beta_1\left(\gamma_2 - \alpha\beta_2\right) + \vec{K}_2\left(\gamma_1\beta_2 - \alpha\beta_1^2\right)}{\Gamma} - \frac{\vec{\tilde{K}}_1\tilde{\beta}_1\left(\tilde{\gamma}_2 - \tilde{\alpha}\beta_2\right) + \vec{\tilde{K}}_2\left(\tilde{\gamma}_1\tilde{\beta}_2 - \tilde{\alpha}\tilde{\beta}_1^2\right)}{\tilde{\Gamma}} \right]^2 +$$

$$\left. + i\vec{\tilde{C}}_1\left(\vec{\tilde{P}}_1 - \vec{\tilde{q}}_1\right) + i\vec{\tilde{C}}_2\left(\vec{\tilde{P}}_2 - \vec{\tilde{q}}_2\right) - i\vec{C}_1\left(\vec{Q} - \vec{q}_1\right) - i\vec{C}_2\left(\vec{Q}_2 - \vec{q}_2\right) \right\},$$

where $\vec{Q}_1$, $\vec{Q}_2$ and $\vec{P}_1$, $\vec{P}_2$ are Jacobi coordinates of oscillator field centres of "bra" and "ket" functions, respectively

$$\vec{Q}_1 = \sqrt{\frac{B_1B_2}{B_1+B_2}}\left(\vec{R}_2 - \vec{R}_1\right), \quad \vec{Q}_2 = \left(B_1+B_2\right)\tilde{\alpha}\left(\vec{R}_3 - \frac{B_1\vec{R}_1 + B_2\vec{R}_2}{B_1+B_2}\right),$$

$$\vec{P}_1 = \sqrt{\frac{A_1 A_2}{A_1+A_2}}\left(\vec{S}_2-\vec{S}_1\right), \qquad \vec{P}_2 = (A_1+A_2)\,\varkappa\left(\vec{S}_3-\frac{A_1\vec{S}_1+A_2\vec{S}_2}{A_1+A_2}\right) \quad (10)$$

Parameters β_1 and γ_1 are expressed through nucleon numbers A_1, A_2 and oscillator radii a_1 and a_2, by formulas (7), and parameters β_2, γ_2, $\varkappa$ and Γ are equal to

$$\beta_2 = \varkappa\left(\frac{A_1}{a_1^2}+\frac{A_2}{a_2^2}-\frac{A_1+A_2}{a_3^2}\right),$$

$$\gamma_2 = \frac{A_1+A_2}{A_1+A_2+A_3}\,\frac{L}{a_3^2}+\varkappa^2\left(\frac{A_1}{a_1^2}+\frac{A_2}{a_2^2}\right), \quad (11)$$

$$\varkappa = \left[\frac{A_3}{(A_1+A_2)(A_1+A_2+A_3)}\right]^{1/2}, \quad \Gamma = \gamma_1\gamma_2-\varkappa^2\beta_1^2.$$

The parameters $\tilde{\beta}_2$, $\tilde{\gamma}_2$, $\tilde{\varkappa}$ and $\tilde{\Gamma}$ marked by tilda are expressed through nucleon numbers B_1, B_2 and B_3 and oscillator radii b_1, b_2 and b_3 for clusters of "bra" functions by formulae (7) and (11) after transfomation $A_i \to B_i$ and $a_i \to b_i$. In formula (9) the following notation

$$Q = \alpha+\frac{A_3}{2b_3^2}+\tilde{\alpha}+\frac{B_3}{2b_3^2}-\frac{\beta_1^2\gamma_2+\beta_2^2\gamma_1-2\varkappa\beta_1^2\beta_2}{2\Gamma}-\frac{\tilde{\beta}_1^2\tilde{\gamma}_2+\tilde{\beta}_2^2\tilde{\gamma}_1-2\tilde{\varkappa}\tilde{\beta}_1^2\tilde{\beta}_2}{2\tilde{\Gamma}}$$

is introduced.

2. GENERATING MATRIX ELEMENTS OF ALGEBRAIC VERSION

In formula (8) $\vec{q}$ and $\vec{\tilde{q}}$ are parametric coordinates of the relative motion and operators $\hat{H}$, $\hat{A}$ produce no action on them. Therefore having averaged (8) in $\vec{q}$ and $\vec{\tilde{q}}$ with the necessary weight functions we obtain the matrix element of the generator coordinate method without the centre-of-mass motion multiplier. To obtain the generating matrix element of the algebraic version of resonating groups the weight functions should generate the oscillator basis

in the coordinate of relative motion. As is known [4] this is the function of the form

$$\exp\left\{-\frac{1}{2}\gamma_0\left[q^2-2(\vec{q}\vec{s})+\frac{1}{2}\tilde{s}^2\right]\right\},$$
$$\exp\left\{-\frac{1}{2}\tilde{\gamma}_0\left[\tilde{q}^2-2(\vec{\tilde{q}}\vec{\tilde{R}})+\frac{1}{2}\tilde{R}^2\right]\right\} \qquad (12)$$

Having multiplied both parts of equality (8) to the right and to the left by the functions (12) and integrated over $\vec{q}$ and $\vec{\tilde{q}}$ we get

$$\langle\vec{R}_1\tilde{\Phi}_1\tilde{\Phi}_2|\hat{H}\hat{A}|\Phi_1\Phi_2\vec{S}\rangle = \frac{1}{(2\pi)^6}\left(\frac{\gamma\cdot\tilde{\gamma}\cdot\omega}{\gamma_0\tilde{\gamma}_0}\right)^{3/2},$$

$$\times\int\ldots\int d\vec{R}\,d\vec{s}\,d\vec{\kappa}\,d\vec{\varkappa}\,\langle\tilde{\Psi}(R)|\hat{H}|\Psi(S)\rangle\exp\left\{i\vec{\kappa}\left(\vec{R}-\vec{\tilde{R}}\right)-i\vec{\varkappa}\left(\vec{S}-\vec{s}\right)+\right. \qquad (13)$$

$$\left.+\frac{1}{4\omega}\left(\frac{\beta\vec{\kappa}}{\gamma}-\frac{\tilde{\beta}\vec{\varkappa}}{\tilde{\gamma}}\right)^2+\frac{\kappa^2}{2}\left(\frac{1}{\gamma}-\frac{1}{\gamma_0}\right)+\frac{\tilde{\kappa}^2}{2}\left(\frac{1}{\tilde{\gamma}}-\frac{1}{\tilde{\gamma}_0}\right)\right\}.$$

For the Hamiltonian with the Gaussian dependence of nucleon-nucleon potential of the central and spin-orbital interactions one manages to realize analytically all integrations in (13). Then if the matrix element of some operator $\hat{H}_0$ on the wave functions of Brinc model has the form

$$\langle\tilde{\Psi}(R)|\hat{H}_0|\Psi(S)\rangle = \exp\left[-aR^2-bS^2+2c(\vec{R}\vec{S})\right] \qquad (14)$$

the generating matrix element of operator $\hat{H}_0$ of the algebraic version equals

$$\langle\vec{R}_1\tilde{\Phi}_1\tilde{\Phi}_2|\hat{H}_0\hat{A}|\Phi_1\Phi_2\vec{S}\rangle = \left(\frac{\gamma\tilde{\gamma}\omega}{\delta\gamma_0\tilde{\gamma}_0}\right)^{3/2}\exp\left[-\tilde{a}\vec{R}^2-\tilde{b}\vec{S}^2+2\tilde{c}(\vec{R}\vec{S})\right], \qquad (15)$$

where

$$\tilde{a}=\frac{1}{\delta}\left\{a-d\left[\frac{\beta^2}{\omega\gamma^2}+2\left(\frac{1}{\gamma}-\frac{1}{\gamma_0}\right)\right]\right\}-\frac{\tilde{\gamma}}{4},$$

$$\tilde{b} = \frac{1}{\delta}\left\{ b - d\left[\frac{\tilde{\beta}^2}{\omega\tilde{\gamma}^2} + 2\left(\frac{1}{\tilde{\gamma}} - \frac{1}{\tilde{\gamma}_0}\right)\right]\right\}^2 - \frac{\chi}{4}$$

$$\tilde{c} = \frac{1}{\delta}\left[c - \frac{d\beta\cdot\tilde{\beta}}{\omega\gamma\tilde{\gamma}}\right], \quad d = ab - c^2$$

$$\delta = 1 - a\left[\frac{\tilde{\beta}^2}{\omega\tilde{\gamma}^2} + 2\left(\frac{1}{\tilde{\gamma}} - \frac{1}{\tilde{\gamma}_0}\right)\right] - b\left[\frac{\beta^2}{\omega\gamma^2} + 2\left(\frac{1}{\gamma} - \frac{1}{\gamma_0}\right)\right] + \tag{16}$$

$$+ 2\frac{c\beta\cdot\tilde{\beta}}{\omega\gamma\tilde{\gamma}} + 2d\left[\frac{\beta^2}{\omega\gamma^2}\left(\frac{1}{\tilde{\gamma}} - \frac{1}{\tilde{\gamma}_0}\right) + \frac{\tilde{\beta}^2}{\omega\tilde{\gamma}^2}\left(\frac{1}{\gamma} - \frac{1}{\gamma_0}\right) + 2\left(\frac{1}{\gamma} - \frac{1}{\gamma_0}\right)\left(\frac{1}{\tilde{\gamma}} - \frac{1}{\tilde{\gamma}_0}\right)\right]$$

If

$$\langle\tilde{\Psi}(\mathcal{R})|\hat{H}|\Psi(S)\rangle = \mathcal{R}^{2n_1} S^{2n_2}\left(\vec{\mathcal{R}}\vec{S}\right)^{n_3}\left(\eta_1 + \eta_2[\vec{\mathcal{R}}\vec{S}]\right)\langle\tilde{\Psi}(\mathcal{R})|\hat{H}_1|\Psi(S)\rangle \tag{17}$$

then

$$\langle\vec{\mathcal{R}}_1\tilde{\Phi}_1\tilde{\Phi}_2|\hat{H}\hat{A}|\Phi_1\Phi_2\vec{S}\rangle = \frac{(-1)^{\ell_1+\ell_2}}{2^{\ell_3}}\frac{d^{\ell_1}}{da^{\ell_1}}\frac{d^{\ell_2}}{db^{\ell_2}}\frac{d^{\ell_3}}{dc^{\ell_3}}\left(\eta_1 + \frac{\eta_2}{\delta}[\vec{\mathcal{R}}\vec{S}]\right)\langle\vec{\mathcal{R}}_1\hat{H}_0\hat{A}|\Phi_1\Phi_2\vec{S}\rangle \tag{18}$$

Formulas (13)-(18) solve in general, the problem of calculating the generating matrix elements of the RGM algebraic version with various oscillator radii of interacting nuclei.

The algorithm suggested for calculating the generating matrix elements allows one to use as intrinsic wave functions of interacting nuclei the wave functions of the generating coordinate method

$$\Phi_i^{(\alpha)} = \hat{A}\sum_{m=1}^{M} b_m^{(\alpha)}\varphi_i(a_m), \tag{19}$$

where

$$\varphi_i(a_m) = \exp\left[-\frac{1}{2a_m^2}\sum_{k=1}^{A_i}\vec{r}_k^{\,2}\right]\chi(\sigma,\tau)$$

Unknown coefficients $b_m^{(\alpha)}$ are defined from a system of linear homogeneous Hill-Whiller equations

$$\sum_{m=1}^{M}\langle\varphi_i(a_n)|\hat{H}_i - E_\alpha|\hat{A}\varphi_i(a_m)\rangle b_m = 0, \tag{20}$$

where $\hat{H}_i$ is the i-th cluster Hamiltonian. Such a choice of intrinsic wave functions leads to a more complete agreement of the latter with the given nucleon-nucleon potential.

Besides the use of intrinsic wave functions such as (19) allows one to take account of their distorsion caused by intereffect of scattering nuclei in the compound nucleus region. For this with the small number of oscillator quanta of relative motion or, which is the same, at small distances between interacting nuclei one should necessarily refuse from factorising the complete wave function of the system into the functions corresponding to asymptotically noninteracting nuclei. Then the wave function of a two-cluster system in expansion into the oscillator basis of relative motion accepts the following schematic form

$$\Psi = \sum_{n=n_{min}}^{N_1} \sum_{m,K}^{M_1 M_2} B_{mK}(n) \varphi_1(a_m) \varphi_2(a_c) |n\rangle + \tag{21}$$
$$+ \sum_{\alpha=1,\beta=1}^{\alpha_{max},\beta_{max}} \left[\sum_{n=N_1+1}^{N_{max}} C_n^{(\alpha,\beta)} \Phi_1^{(\alpha)} \Phi_2^{(\beta)} |n\rangle + \sum_{n=N_{max}+1}^{\infty} C_n^{(\alpha,\beta)} \Phi_1^{(\alpha)} \Phi_2^{(\beta)} |n\rangle \right],$$

where $C_n^{(\alpha,\beta)}$ are asymptotic coefficients determined by the energy and the quantum numbers of the system [3]. $B_{mK}(n)$ and $C_n^{(\alpha,\beta)}$ are coefficieints that should be defined by solving a system of the type (1) linear equations under the given boundary conditions on infinity.

The novelty of this approach as compared with the known ones for the RGM algebraic version is in the first sum in (21) which describes the distorsion of intrinsic wave functions of the nuclei caused by their interaction.

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Received February 15, 1986.

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Семен Абрамович Бадалов
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Производящие матричные элементы гамильтониана алгебраической версии метода резонирующих групп на внутренних волновых функциях с различными осцилляторными длинами

Редактор А.А.Храброва Техн.редактор Л.П.Львова
Зак. 216 Формат 60x84/16. Уч.-изд.л. 0,5
Подписано к печати 21.02.1986 года. Тираж 200. Цена 4 коп.
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