SINGLE-PARTICLE BASIS AND TRANSLATIONAL INVARIANCE IN THE MICROSCOPIC APPROACH TO NUCLEAR REACTIONS

V. D. EFROS

I. V. Kurchatov Atomic Energy Institute, Moscow*

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A method of practically solving of nuclear reaction problems on a single-particle basis is proposed within the framework of the microscopic approach. The method ensures the fulfilment of Pauli's principle and translational invariance requirements.

The results of recent "model" nuclear reaction calculations proceeding from a given NN interaction (see e.g. Ref. [1]), lead perhaps to a conclusion that if the corresponding "rigorous" calculations were performed in some cases satisfactory results would be obtained without using an anrealistically great number of basis states. The difficulty in performing such calculations is mainly in the typical "mixing" of NN force operators and of different-type fragment Ψ-functions in the corresponding many-particle cluster matrix elements (m.e.). This does not permit the variable separation in the m.e. Direct numerical integration is practical only for $A = 3$ in the unrealistic case of purely static NN potentials. The method of the calculation in Ref. [2] deals with the intrinsic (Jacobi) coordinates $\{\zeta\}$ and therefore it could be efficient only for small A; the methods in Refs [3, 4] involve uncontrollable model-type approximations that are not in accordance with the initial idea of the microscopic calculation. The method given below does not require such approximations.

Let $\varphi(\{\xi\})$ be the Ψ-function to be found in the reaction problem. Let us consider the "extended" Ψ-function instead of $\varphi(\{\xi\})$:

$$\overline{\Psi} = \varphi(\{\xi\})\chi_{N=L=M=0}(\boldsymbol{R}_{\text{C.M.}}A^{1/2}/B), \tag{1}$$

where χ_{NLM} are oscillator functions, $\boldsymbol{R}_{\text{C.M.}}$ is the centre-of-mass coordinate, $B/A^{1/2}$ is the oscillator radius. Instead of the initial equation $(H-\mathscr{E})\varphi = 0$ in the $\{\xi\}$-subspace, H being the intrinsic hamiltonian, we shall solve the equation $(H-\mathscr{E})\overline{\Psi} = 0$ in the whole $\{\boldsymbol{r}\}$-space and we shall seek for $\overline{\Psi}$ in the form

$$\overline{\Psi} = (\sum_{\gamma} c_{\gamma}\mathscr{A}F_{\gamma})\chi_{000}(\boldsymbol{R}_{\text{C.M.}}A^{1/2}/B) + \overline{\Psi}_{\text{loc}}. \tag{2}$$

* Address: I. V. Kurchatov Atomic Energy Institute, Kurchatov Square, Moscow D-182, USSR.

Here the coefficients c_γ correspond to the unknown reaction amplitudes, F_γ are cluster functions of the type

$$F_\gamma = \varphi_{1\gamma}(\{\xi^{1\gamma}\})\varphi_{2\gamma}(\{\xi^{2\gamma}\})f_\gamma(\varrho_\gamma)Y_{L_\gamma M_\gamma}(\hat{\varrho}_\gamma), \tag{3}$$

where $\varphi_{1\gamma,2\gamma}$ are the intrinsic Ψ-functions of the fragments participating in the reaction, f_γ is their relative motion function, $\varrho_\gamma = \boldsymbol{R}^{2\gamma}_{\text{C.M.}} - \boldsymbol{R}^{1\gamma}_{\text{C.M.}}$. All the functions in Eq. (3) depend on Jacobi coordinates but below we shall be able to avoid calculations with these coordinates. $\mathscr{A}$ in Eq. (2) is the antisymmetrization operator, $\overline{\Psi}_{\text{loc}}$ is a normalizable function. We construct $\overline{\Psi}_{\text{loc}}$ as an expansion

$$\overline{\Psi}_{\text{loc}} = \sum_\mu c_\mu \psi_\mu(\{\boldsymbol{r}_K\}) \tag{4}$$

with ψ_μ being single-particle oscillator configurations. We retain in the expansion all the configurations (with given J, T) of a shell. Then, as can be easily seen when using either usual Hulthén-Kohn-type equations

$$\langle\psi_\mu|\,[H-\mathscr{E}]\rangle\overline{\Psi} = 0, \quad \langle F_{\gamma'}|\,[H-\mathscr{E}]\overline{\Psi}\rangle = 0, \tag{5}$$

or similar equations (cf. Ref. [2]) for obtaining unknown c_γ from Eq. (2) and c_μ from Eq. (4), the resultant $\overline{\Psi}_{\text{loc}}$, Eq. (4), will be in fact of the factorized form of Eq. (1) type; so the required factorization of $\overline{\Psi}$, Eq. (1), will be exact. The factorized ("pure in the centre-of-mass") ψ_μ configuration combinations constructed beforehand in a familiar way may be used as well.

For solving Eqs (5) all we have to do in addition to boundstate-type calculations, reducing mainly to the calculation of the two-particle m.e. of the type

$$\int d\boldsymbol{r}_1 d\boldsymbol{r}_2 g_a^*(\boldsymbol{r}_1)g_b^*(\boldsymbol{r}_2)\hat{V}(12)g_c(\boldsymbol{r}_1)g_d(\boldsymbol{r}_2), \tag{6}$$

is to calculate the m.e. with the cluster functions (3) of the type

$$\langle\psi_\mu|[H-\mathscr{E}]F_\gamma\chi_{000}\rangle, \tag{7a}$$

$$\langle\mathscr{A}F_{\gamma'}\chi_{000}|[H-\mathscr{E}]F_\gamma\chi_{000}\rangle. \tag{7b}$$

We may write in Eqs (7)

$$[H-\mathscr{E}]F_\gamma\chi_{000} = \hat{V}_{\text{int}}F_\gamma\chi_{000} + \tilde{F}_\gamma\chi_{000}, \tag{8}$$

where $\hat{V}_{\text{int}}$ is the inter-cluster NN interaction sum, $\tilde{F}_\gamma = (T_{\text{rel}} - \mathscr{E}_{\text{rel}})F_\gamma$. The function $\tilde{F}_\gamma$ corresponds to replacing $f_\gamma(\varrho_\gamma)$ from F_γ by some localized $\tilde{f}_\gamma(\varrho_\gamma)$. Further, as it is discussed in Refs [2, 3] in the framework of quite different approaches, we may replace relative motion functions by the finite sums of the oscillator functions after putting (8) into (7).[1] Let us do it by using $(A/A_{1\gamma}A_{2\gamma})^{1/2}B$ ($A_{1\gamma,\,2\gamma}$ are the fragment nucleon numbers) as an oscillator radius in the corresponding expansions:

$$f_\gamma(\varrho_\gamma)Y_{L_\gamma M_\gamma}(\hat{\varrho}_\gamma) \to \sum_N c^\gamma_N \chi_{NL_\gamma M_\gamma}(\varrho_\gamma(A_{1\gamma}A_{2\gamma}/A)/B) \tag{9}$$

[1] It is useful to make beforhand a cutting of the functions $f_\gamma, f_{\gamma'}$ at distances greater than the fragment interaction region [2]. Below without changing notation we may consider it fulfilled.

and the same for $f_{\gamma'}$, $\tilde{f}_{\gamma}$. The coordinates $\boldsymbol{R}_{\text{C.M.}}A^{1/2}$, $\varrho_\gamma(A_{1\gamma}A_{2\gamma}/A)^{1/2}$ are related to the fragment center-of-mass coordinates $\boldsymbol{R}^{1\gamma}_{\text{C.M.}}A^{1/2}_{1\gamma}$, $\boldsymbol{R}^{2\gamma}_{\text{C.M.}}A^{1/2}_{2\gamma}$ by means of an orthogonal transformation. Making use of it we transform the oscillator function products:

$$\chi_{000}(\boldsymbol{R}_{\text{C.M.}}A^{1/2}/B)\chi_{NL_\gamma M_\gamma}(\varrho_\gamma(A_{1\gamma}A_{2\gamma}/A)^{1/2}/B) = \sum_{2n_1+l_1+2n_2+l_2=2N+L_\gamma}(-1)^{L_\gamma}$$

$$\times\langle n_1 l_1 n_2 l_2|00NL_\gamma\rangle^{\varphi}_{L_\gamma}[\chi_{n_1 l_1 m_1}(\boldsymbol{R}^{1\gamma}_{\text{C.M.}}A^{1/2}_{1\gamma}/B)\chi_{n_2 l_2 m_2}(\boldsymbol{R}^{2\gamma}_{\text{C.M.}}A^{1/2}_{2\gamma}/B)]_{L_\gamma M_\gamma}. \tag{10}$$

Here $\langle\ldots|\ldots\rangle^{\varphi}_{L\gamma}$ are the generalized oscillator brackets of a quite simple special type (see e.g. [5]). But the products of the type

$$\varphi_{1\gamma}(\{\xi^{1\gamma}\})\chi_{n_1 l_1 m_1}(\boldsymbol{R}_{1\gamma}A^{1/2}_{1\gamma}/B),\ \varphi_{2\gamma}(\{\xi^{2\gamma}\})\chi_{n_2 l_2 m_2}(R_{2\gamma}A^{1/2}_{2\gamma}/B) \tag{11}$$

just can be simply expressed in the single-particle form by means of their expansions of the type

$$\sum_\mu c_\mu(n_1 l_1 m_1)\psi_\mu(\{\boldsymbol{r}_{k'}\}),\ \sum_\mu c_\mu(n_2 l_2 m_2)\psi_\mu(\{\boldsymbol{r}_{k''}\}). \tag{12}$$

Indeed, for $n = l = m = 0$ case they (i.e. $c_\mu(000)$) can be found by solving bound-state problems with a usual pure in the centre-of-mass oscillator-configuration-combination basis. The remaining functions (12) can be obtained from $c_\mu(000)$ with the help of the following recurrence:

$$c_\mu(0lm) = l^{-1/2}\sum_{m'=0,\pm1} C^{lm}_{1m'l-1m-m'}\sum_{\mu'}\langle\psi_\mu|\eta_{m'}|\psi_{\mu'}\rangle c_{\mu'}(0\ l-1\ m-m') \tag{13a}$$

and then with given l:

$$c_\mu(nlm) = -[2n(2n+2l+1)]^{-1/2}\sum_{\mu'}\langle\psi_\mu|\boldsymbol{\eta}^2|\psi_{\mu'}\rangle c_{\mu'}(n-1lm). \tag{13b}$$

Here $\eta = 2^{-1/2}(x-\partial/\partial x)$ are the creation operators in the centre-of-mass variables ($x_i = \boldsymbol{R}^{iy}_{\text{C.M.}}A^{1/2}_{iy}/B$). For calculating the m.e. (13) we shall use the relations

$$\boldsymbol{\eta} = A^{-1/2}\sum_{k=1}^{A}\boldsymbol{a}_k;\qquad \boldsymbol{a}_k = 2^{-1/2}(B^{-1}\boldsymbol{r}_k - B\partial/\partial\boldsymbol{r}_k);$$

$$\boldsymbol{\eta}^2 = \sum_{k=1}^{A}\boldsymbol{a}_k^2 - A^{-1}\sum_{1\leqslant k<j<A}(\boldsymbol{a}_j-\boldsymbol{a}_k)^2 \tag{14}$$

so in every step of the recurrence one must calculate only single and two-particle m.e. As it is seen from Eqs (14) only $\psi_{\mu'}$ contiguous to ψ_μ contribute to the sums over μ' in Eqs (13).

All the Ψ-functions in the m.e. (7) are now reduced to the determinants $\psi_\mu(\{\boldsymbol{r}_k\})$ and to the products $\psi_{\mu_1}(\{\boldsymbol{r}_{k'}\})\psi_{\mu_2}(\{\boldsymbol{r}_{k''}\})$ of the fragment determinants. The quantities $\mathscr{A}\psi_{\mu_1}(\{\boldsymbol{r}_{k'}\})\psi_{\mu_2}(\{\boldsymbol{r}_{k''}\})$ arising in (7b) are then obviously exactly as the determinants of the type $\psi_\mu(\{\boldsymbol{r}_k\})$ so the m.e. (7b) is reduced to the sum of the m.e. (7a)[2]. The m.e. (7a)

[2] Here there is some resemblance to calculations [6, 3] based on intrinsic functions dependent on Jacobi coordinates.

themselves are reduced to a m.e. sum of the type (if the nucleon with number 1 is assumed to be in $\varphi_{1\gamma}$ and that with number 2 in $\varphi_{2\gamma}$:

$$\int d\tau_{r_k} \psi_\mu^*(\{r_k\}) \hat{V}(12) \psi_{\mu_1}(\{r_{k'}\}) \psi_{\mu_2}(\{r_{k''}\}),$$

$$\int d\tau_{r_k} \psi_\mu^*(\{r_k\}) \psi_{\mu_1}(\{r_{k'}\}) \psi_{\mu_2}(\{r_{k''}\}).$$

The second m.e. is quite simple and the first one also reduces directly to the ordinary two-particle m.e. (6). The generalization to orbitals different from the oscillator ones is also possible.

A note concerning m.e. (7b) should also be made. These m.e. arise in the equations with $F_{\gamma'}$ from Eqs (5). The way used above of calculating them means replacing $\chi_{000}F_{\gamma'}$ in (7b) by

$$[\chi_{000}F_{\gamma'}]_{\mu_0} = \sum_{\mu \leqslant \mu_0} \langle \psi_\mu | \chi_{000}F_{\gamma'} \rangle \psi_\mu(\{r_k\}).$$

Note that in addition to this, it is useful to make the replacement in every m.e. in the equations. That means to replace the equations by

$$\langle [\chi_{000}F_{\gamma'}]_{\mu_0} | [H - \mathscr{E}] \bar{\Psi} \rangle = 0. \tag{15}$$

This procedure preserves the projectional character of the equations and consequently the results would not be sensitive to the difference between $\chi_{000}F_{\gamma'}$ and $[\chi_{000}F_{\gamma'}]_{\mu_0}$.

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