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UNIVERSAL COORDINATE GAUSSIAN BASIS FOR CALCULATIONS OF THE BOUND STATES OF A FEW-PARTICLE SYSTEM

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A new simple basis is proposed for variational calculations of the bound states of a few-particle system. For an N-particle system with pairwise interactions, the matrix elements of the Hamiltonian are found in an explicit form. A modified version of the basis invariant with respect to spatial translations is considered as well. As an example, the ^{12}C nucleus is considered as a system consisting of three α-particles, and the convergence of the method is briefly discussed.

K e y w o r d s: a few-body system, variational method, variational basis.

1. Introduction

To carry on variational calculations, it is suitable to expand the trial wave function in a series of basic functions. Then the Schrödinger equation becomes a system of linear algebraic ones. For variational calculations, different bases are used, as well as their combinations. One of the most popular is the oscillator-type basis [1–3], although the calculation of the matrix elements for basic functions with high quantum numbers is a nontrivial procedure [4, 5]. The usage of the Gaussian basis [6, 7] in calculations of the main characteristics and the structure of a few-body system has proved its efficiency in a number of studies of three-body [8–10], four-body [11–13], five-body [14–16] and even more complicated systems. Some modifications [17] of this basis were proposed to enhance the efficiency of calculations.

In the present work, we propose a new version of the basis for expanding the trial wave function within the variational calculations. It seems to be more simple, but also efficient enough to treat few-particle systems with high precision. Its specific feature is that the trial wave function with any angular momentum and permutational symmetry may be expanded into the series in such basic functions without additional projection onto a definite state. After solving the variational problem, the angular momentum and permutational symmetry of the given state can be found having the wave function in a simple and explicit form.

We consider two modifications of the basis, with and without translation invariance. We obtain the explicit expressions for matrix elements of the kinetic energy operator, for the potential operator having the form of a sum of Gaussian pairwise functions, as well as for the Coulomb pair interaction potentials. In order to make the formulae less complicated, we consider a three-particle system when calculating the matrix elements of the kinetic and potential energies. But, the obtained expressions can be trivially and directly generalized to the N-particle case. Finally, we consider a model of ^{12}C nucleus as a system of three α-particles in order to estimate the convergence of the method.

2. Statement of the Problem

For simplicity, consider a three-particle system. Let the Hamiltonian of the system

$$\hat{H} = -\frac{\hbar^2}{2m_1}\triangle_1 - \frac{\hbar^2}{2m_2}\triangle_2 - \frac{\hbar^2}{2m_3}\triangle_3 + \\ + V_{12}(r_{12}) + V_{13}(r_{13}) + V_{23}(r_{23}) + \frac{\hbar^2}{2M}\triangle_{\text{c.m.}}, \quad (1)$$

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contain, in addition to the kinetic energy, the pairwise potentials depending on the relative distances $r_{jk} \equiv |\mathbf{r}_j - \mathbf{r}_k|$. In Hamiltonian (1), we explicitly extract the kinetic energy of the center of mass ($M = m_1 + m_2 + m_3$ is the total mass of the system).

Now, we assume that the trial wave function of the system can be expanded in terms of the basic functions of two different forms: the first one is a simple superposition of the products of one-particle Gaussian functions,

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \sum_{k=1}^{K} C_k \varphi_k(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3), \tag{2}$$

where

$$\varphi_k(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \equiv \exp\left(-\sum_{j=1}^{3} a_{jk} (\mathbf{r}_j - \mathbf{R}_{jk})^2\right) \equiv$$

$$\equiv \prod_{j=1}^{3} \exp\Big(-a_{jk} (\mathbf{r}_j - \mathbf{R}_{jk})^2\Big), \tag{3}$$

and C_k are the coefficients of the expansion. In (3), the parameters a_{jk} and $\mathbf{R}_{jk}$ are the variational parameters (generally speaking, they may be complex numbers). We impose the additional condition onto the parameters $\mathbf{R}_{jk}$:

$$\sum_{j=1}^{3} m_j \mathbf{R}_{jk} = 0, \quad k = 1, 2, ..., K. \tag{4}$$

Due to this or any other similar relation, the possible many-valuedness of the parameters $\mathbf{R}_{jk}$ due to arbitrary spatial translations is eliminated. On the other hand, we do not impose any relations to avoid the ambiguity of the same parameters with respect to the rotations in the three-dimensional space. Thus, the wave functions obtained in the variational calculations can be found in different equivalent forms which differ one from another only by a rotation in space.

Note that, in the case of an N-particle system, the upper limit in the sum and the product of expression (3) should be changed by N.

The second version of the basis to be considered is the following:

$$\Phi(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3) = \sum_{k=1}^{K} C_k \psi_k(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3), \tag{5}$$

where $\tilde{\mathbf{r}}_j \equiv \mathbf{r}_j - \mathbf{R}_{\text{c.m.}}$, and the basic functions

$$\psi_k(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3) \equiv \exp\left(-\sum_{j=1}^{3} a_{jk} (\tilde{\mathbf{r}}_j - \mathbf{R}_{jk})^2\right) \equiv$$

$$\equiv \prod_{j=1}^{3} \exp\Big(-a_{jk} (\tilde{\mathbf{r}}_j - \mathbf{R}_{jk})^2\Big). \tag{6}$$

The difference between ψ_k from (6) and φ_k from (3) lies in the fact that $\psi_k(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3)$ does not depend on the coordinate of the center of mass of the system in the Jacobi coordinates. Each basic function depends only on two Jacobi coordinates, and it is invariant with respect to translations of the system in space. In all the matrix elements, the integrals imply the integration only over two Jacobi coordinates.

To find the coefficients C_k of expansion (2) for the total wave function, we can use the variational principle in the form of the Galerkin method. This means a solution of the system of algebraic equations

$$\sum_{k=1}^{K} C_k \left\langle \varphi_n \left| \hat{H} - E \right| \varphi_k \right\rangle = 0, \quad n = 1, ..., K. \tag{7}$$

When $K \to \infty$, system (7) becomes equivalent to the Schrödinger equation under the condition that the basis is complete.

It is obvious that, in the case of basis (6), one has to solve a system of equations similar to (7), but with matrix elements calculated with the use of ψ_k.

3. Calculation of Matrix Elements

We start to calculate the matrix elements from (7). Let us begin with the matrix elements for the first version of the basis φ_k given by expression (3). In particular, the normalization

$$\langle \varphi_n | \varphi_k \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \, \varphi_n^*(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \, \varphi_k(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) =$$

$$= \prod_{j=1}^{3} \int d\mathbf{r} \exp\Big(-a_{jn}(\mathbf{r} - \mathbf{R}_{jn})^2 - a_{jk}(\mathbf{r} - \mathbf{R}_{jk})^2\Big) =$$

$$= \prod_{j=1}^{3} \left(\frac{\pi}{u_{j,nk}}\right)^{3/2} \exp\Big(-A_{j,nk} (\mathbf{R}_{jn} - \mathbf{R}_{jk})^2\Big), \tag{8}$$

where

$$u_{j,nk} \equiv a_{jn} + a_{jk}, \quad A_{j,nk} \equiv \frac{a_{jn} a_{jk}}{a_{jn} + a_{jk}}. \tag{9}$$

It is obvious that, for an N-particle system, the product in (8) should be simply spread from 1 to N.

The kinetic energy matrix element (consider a particle number j):

$$\left\langle\varphi_n\left|-\frac{\hbar^2}{2m_j}\triangle_j\right|\varphi_k\right\rangle =$$

$$=\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \varphi_n^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\left(-\frac{\hbar^2}{2m_j}\triangle_j\right)\varphi_k(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=$$

$$=\int d\mathbf{r}_j\, e^{-a_{jn}(\mathbf{r}_j-\mathbf{R}_{jn})^2}\left(-\frac{\hbar^2}{2m_j}\triangle_j\right)e^{-a_{jk}(\mathbf{r}_j-\mathbf{R}_{jk})^2}\times$$

$$\times\prod_{s\neq j}\left(\frac{\pi}{u_{s,nk}}\right)^{3/2} e^{-Q_{s,nk}} =$$

$$=\frac{\hbar^2}{2m_j}A_{j,nk}\cdot(6-4Q_{j,nk})\prod_{s=1}^{3}\left(\frac{\pi}{u_{s,nk}}\right)^{3/2} e^{-Q_{s,nk}}, \quad (10)$$

where

$$Q_{s,nk}\equiv A_{s,nk}\left(\mathbf{R}_{sn}-\mathbf{R}_{sk}\right)^2. \quad (11)$$

We can easily find that, in the N-particle case, the product in (10) should be simply spread from 1 to N.

We assume (for simplicity) that the pair potentials in Hamiltonian (1) are superpositions of a few Gaussian functions,

$$V_{ij}\left(r_{ij}\right)=\sum_s \mathcal{V}_s\exp\left(-b_s r_{ij}^2\right). \quad (12)$$

In this case, the matrix elements for the potential energy can be calculated in an explicit form. Consider one of the terms from the sum

$$\langle\varphi_n|V_{ij}|\varphi_k\rangle=\sum_s \mathcal{V}_s\left\langle\varphi_n\left|\exp\left(-b_s r_{ij}^2\right)\right|\varphi_k\right\rangle, \quad (13)$$

Let $i=1$, $j=2$. We have

$$\left\langle\varphi_n\left|\exp\left(-b_s r_{12}^2\right)\right|\varphi_k\right\rangle =$$

$$=\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3\,\varphi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\,e^{-b_s r_{12}^2}\,\varphi\left(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3\right)=$$

$$=\left(\frac{\pi}{u_{3,nk}}\right)^{3/2} e^{-Q_{3,nk}}\int d\mathbf{r}_1 d\mathbf{r}_2\, e^{-F_{nk}(\mathbf{r}_1,\mathbf{r}_2)}. \quad (14)$$

In (14), we denoted the quadratic form

$$F_{nk}\left(\mathbf{r}_1,\mathbf{r}_2\right)\equiv a_{1n}\left(\mathbf{r}_1-\mathbf{R}_{1n}\right)^2+a_{1k}\left(\mathbf{r}_1-\mathbf{R}_{1k}\right)^2+$$

$$+a_{2n}\left(\mathbf{r}_2-\mathbf{R}_{2n}\right)^2+a_{2k}\left(\mathbf{r}_2-\mathbf{R}_{2k}\right)^2+b_s\left(\mathbf{r}_2-\mathbf{r}_1\right)^2. \quad (15)$$

After the explicit integration in (14), we have

$$\left\langle\varphi_n\left|\exp\left(-b_s r_{12}^2\right)\right|\varphi_k\right\rangle=\frac{\pi^{9/2}\,e^{-Q_{3,nk}-P_{12,nk}}}{\left(u_{3,nk}D_{12,nk}\right)^{3/2}}, \quad (16)$$

where

$$D_{12,nk}\equiv u_{1,nk}u_{2,nk}+b_s(u_{1,nk}+u_{2,nk}), \quad (17)$$

$$P_{12,nk}\equiv(u_{1,nk}+b_s)q_1^2+(u_{2,nk}+b_s)q_2^2-2b_s(\mathbf{q}_1\mathbf{q}_2)-$$

$$-2\left(\mathbf{q}_1\mathbf{p}_1\right)-2\left(\mathbf{q}_2\mathbf{p}_2\right)+$$

$$+a_{1n}R_{1n}^2+a_{1k}R_{1k}^2+a_{2n}R_{2n}^2+a_{2k}R_{2k}^2. \quad (18)$$

In expression (18), we used the following denotations:

$$\begin{aligned}
&\mathbf{p}_1\equiv a_{1n}\mathbf{R}_{1n}+a_{1k}\mathbf{R}_{1k},\\
&\mathbf{p}_2\equiv a_{2n}\mathbf{R}_{2n}+a_{2k}\mathbf{R}_{2k},\\
&\mathbf{q}_1\equiv\frac{u_{2,nk}\mathbf{p}_1+b_s\left(\mathbf{p}_1+\mathbf{p}_2\right)}{D_{12,nk}},\\
&\mathbf{q}_2\equiv\frac{u_{1,nk}\mathbf{p}_2+b_s\left(\mathbf{p}_1+\mathbf{p}_2\right)}{D_{12,nk}}.
\end{aligned} \quad (19)$$

It is obvious that, in the case of N-particle system, expression (16) can be trivially generalized: instead of expression $\left(\frac{\pi}{u_{3,nk}}\right)^{3/2}e^{-Q_{3,nk}}$, we have to put the product $\prod_{s=3}^{N}\left(\frac{\pi}{u_{s,nk}}\right)^{3/2}e^{-Q_{s,nk}}$.

Now, we have to calculate the matrix element from the kinetic energy of the center of mass of the system:

$$\left\langle\varphi_n\left|-\frac{\hbar^2}{2M}\triangle_{\text{c.m.}}\right|\varphi_k\right\rangle =$$

$$=-\frac{\hbar^2}{2M}\int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3\varphi_n^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)\triangle_{\text{c.m.}}\varphi_k(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3). \quad (20)$$

Introducing the Jacobi coordinates,

$$\begin{aligned}
&\mathbf{r}\equiv\mathbf{r}_2-\mathbf{r}_1,\\
&\boldsymbol{\rho}\equiv\mathbf{r}_3-\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2}{m_1+m_2},\\
&\mathbf{R}_{\text{c.m.}}\equiv\mathbf{R}\equiv\frac{m_1\mathbf{r}_1+m_2\mathbf{r}_2+m_3\mathbf{r}_3}{m_1+m_2+m_3},
\end{aligned} \quad (21)$$

or the inverse relations

$$\mathbf{r}_1\equiv\mathbf{R}-\frac{m_3}{M}\boldsymbol{\rho}-\frac{m_2}{m_1+m_2}\mathbf{r},$$

$$\mathbf{r}_2 \equiv \mathbf{R} - \frac{m_3}{M}\boldsymbol{\rho} + \frac{m_1}{m_1+m_2}\mathbf{r},$$
$$\mathbf{r}_3 \equiv \mathbf{R} + \frac{m_1+m_2}{M}\boldsymbol{\rho}, \tag{22}$$

we have

$$\left\langle \varphi_n \middle| -\frac{\hbar^2}{2M}\triangle_R \middle| \varphi_k \right\rangle =$$
$$= \int d\mathbf{r}\, d\boldsymbol{\rho}\, d\mathbf{R}\, \varphi_n^*(\mathbf{r},\boldsymbol{\rho},\mathbf{R})\left(-\frac{\hbar^2}{2M}\triangle_R\right)\varphi_k(\mathbf{r},\boldsymbol{\rho},\mathbf{R}) =$$
$$= \frac{\hbar^2}{2M}\int d\mathbf{r}\, d\boldsymbol{\rho}\, d\mathbf{R}\, (\nabla_R\, \varphi_n^*(\mathbf{r},\boldsymbol{\rho},\mathbf{R}), \nabla_R\, \varphi_k(\mathbf{r},\boldsymbol{\rho},\mathbf{R})). \tag{23}$$

Omitting the details of the trivial cumbersome operations of differentiation and integration, we get

$$\left\langle \varphi_n \middle| -\frac{\hbar^2}{2M}\triangle_R \middle| \varphi_k \right\rangle = \frac{\hbar^2}{2M}\prod_{q=1}^{3}\left(\left(\frac{\pi}{u_{q,nk}}\right)^{3/2} e^{-Q_{q,nk}}\right) \times$$
$$\times \left(6\sum_{j=1}^{3} A_{j,nk} - 4\sum_{s,p=1}^{3} A_{s,nk}A_{p,nk}\,(\mathbf{R}_{sn}-\mathbf{R}_{sk}, \mathbf{R}_{pn}-\mathbf{R}_{pk})\right). \tag{24}$$

The denotations used in (24) are given above. We also note that, in the case of N-particle system, we have to spread the upper limit in the sums and in the product of expression (24) to N (instead of 3).

Very often, we deal with the Coulomb interaction between particles. Let us consider such an interaction (between particles 1 and 2, for example):

$$V_C\,(r_{12}) = \frac{Z_1 Z_2 e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}. \tag{25}$$

In expression (25), $Z_1 e$ and $Z_2 e$ are the charges of particles 1 and 2, respectively, and e is the elementary charge ($e^2 = 1.4399764$ MeV $\cdot$ fm). Let us calculate the expression for the matrix element for potential (25):

$$\langle \varphi_n | V_C\,(r_{12}) | \varphi_k \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3\, \varphi^* V_C(r_{12})\, \varphi =$$
$$= \frac{\pi^{3/2}}{u_{3,nk}^{3/2}} e^{-Q_{3,nk}} \int d\mathbf{r}_1 d\mathbf{r}_2 \prod_{s=1}^{2} e^{-a_{sn}(\mathbf{r}_s - \mathbf{R}_{sn})^2} V_C(r_{12}) \times$$
$$\times \prod_{q=1}^{2} e^{-a_{qk}(\mathbf{r}_q - \mathbf{R}_{qk})^2}. \tag{26}$$

After the transition to new variables $\mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2$ and $\boldsymbol{\rho} \equiv \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2)$, we have, instead of (26),

$$\langle \varphi_n | V_C\,(r_{12}) | \varphi_k \rangle = \frac{\pi^{3/2} e^{-Q_{3,nk}}}{u_{3,nk}^{3/2}} \frac{\pi^{3/2} e^{-Y_{12,nk}}}{(u_{1,nk}+u_{2,nk})^{3/2}} \times$$
$$\times \int d\mathbf{r}\, V_C(r) \exp\left(-\left(U_{12,nk}\, r^2 + 2\,(\mathbf{r}\cdot\mathbf{T}_{12,nk})\right)\right), \tag{27}$$

where

$$U_{12,nk} \equiv \frac{u_{1,nk}u_{2,nk}}{u_{1,nk}+u_{2,nk}}, \tag{28}$$

$$\mathbf{T}_{12,nk} \equiv \frac{u_{1,nk}\,(a_{2n}\mathbf{R}_{2n} + a_{2k}\mathbf{R}_{2k})}{u_{1,nk}+u_{2,nk}} -$$
$$- \frac{u_{2,nk}\,(a_{1n}\mathbf{R}_{1n} + a_{1k}\mathbf{R}_{1k})}{u_{1,nk}+u_{2,nk}}, \tag{29}$$

$$Y_{12,nk} \equiv \frac{a_{1n}a_{1k}\,(\mathbf{R}_{1n}-\mathbf{R}_{1k})^2 + a_{2n}a_{2k}\,(\mathbf{R}_{2n}-\mathbf{R}_{2k})^2}{u_{1,nk}+u_{2,nk}} +$$
$$+ \frac{a_{1n}a_{2n}\,(\mathbf{R}_{1n}-\mathbf{R}_{2n})^2 + a_{1k}a_{2k}\,(\mathbf{R}_{1k}-\mathbf{R}_{2k})^2}{u_{1,nk}+u_{2,nk}} +$$
$$+ \frac{a_{1n}a_{2k}\,(\mathbf{R}_{1n}-\mathbf{R}_{2k})^2 + a_{1k}a_{2n}\,(\mathbf{R}_{1k}-\mathbf{R}_{2n})^2}{u_{1,nk}+u_{2,nk}}. \tag{30}$$

Taking into account that

$$\int \frac{d\mathbf{r}}{r} e^{-\left(Ar^2 + 2(\mathbf{r}\cdot\mathbf{B})\right)} = \frac{\pi^{3/2} e^{\frac{B^2}{A}}}{|\mathbf{B}|\sqrt{A}} \operatorname{erf}\left(\frac{|\mathbf{B}|}{\sqrt{A}}\right), \tag{31}$$

we obtain, instead of (27),

$$\langle \varphi_n | V_C\,(r_{12}) | \varphi_k \rangle = \frac{\pi^{3/2} e^{-Q_{3,nk}}}{u_{3,nk}^{3/2}} \frac{\pi^{3/2} e^{-Y_{12,nk}}}{(u_{1,nk}+u_{2,nk})^{3/2}} \times$$
$$\times \frac{Z_1 Z_2 e^2 \pi^{3/2} e^{X_{12,nk}^2}}{P_{12,nk}} \operatorname{erf}(X_{12,nk}), \tag{32}$$

where

$$X_{12,nk} \equiv \frac{|\mathbf{T}_{12,nk}|}{\sqrt{U_{12,nk}}}, \quad P_{12,nk} \equiv |\mathbf{T}_{12,nk}|\sqrt{U_{12,nk}}, \tag{33}$$

and $\operatorname{erf}(x)$ is the well-known function

$$\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \tag{34}$$

Note at last that, in the case of N-particle system, one has to change the very first fraction in expression (32) by the product of such fractions from $j = 3$ to

$j = N$ and to insert the subindex j instead of the fixed subindex 3 in the above-mentioned fraction.

Now, let us give the expressions for matrix elements in the case of basis (6) which is invariant with respect to the spatial translations. Here, we restrict ourselves with a three-particle case. Further, we use the notation $\psi_k(\mathbf{r}, \boldsymbol{\rho})$ of the basic functions with the arguments $\mathbf{r}$ and $\boldsymbol{\rho}$ being the Jacobi coordinates. The normalization matrix element

$$\langle \psi_n | \psi_k \rangle = \int d\mathbf{r}\, d\boldsymbol{\rho}\, \psi_n^*(\mathbf{r}, \boldsymbol{\rho})\, \psi_k(\mathbf{r}, \boldsymbol{\rho}) =$$

$$= \int d\mathbf{r} d\boldsymbol{\rho} e^{-\left(G_{11}\rho^2 + 2G_{12}(\boldsymbol{\rho},\mathbf{r}) + G_{22}r^2 + 2(\boldsymbol{\rho},\mathbf{Y}_1) + 2(\mathbf{r},\mathbf{Y}_2) + S\right)}, \quad (35)$$

where

$$G_{11} \equiv \frac{1}{M^2}\left(m_3^2\,(u_{1,nk} + u_{2,nk}) + (m_1 + m_2)^2\, u_{3,nk}\right),$$

$$G_{22} \equiv \frac{1}{(m_1 + m_2)^2}\left(m_2^2\, u_{1,nk} + m_1^2\, u_{2,nk}\right),$$

$$G_{12} \equiv \frac{m_3}{M\,(m_1 + m_2)}(m_2\, u_{1,nk} - m_1\, u_{2,nk}),$$

$$\mathbf{Y}_1 \equiv \frac{1}{M}(m_3(a_{1n}\mathbf{R}_{1n} + a_{1k}\mathbf{R}_{1k} + a_{2n}\mathbf{R}_{2n} + a_{2k}\mathbf{R}_{2k}) -$$

$$- (m_1 + m_2)\,(a_{3n}\mathbf{R}_{3n} + a_{3k}\mathbf{R}_{3k})),$$

$$S \equiv \sum_{j=1}^{3}\left(a_{jn}R_{jn}^2 + a_{jk}R_{jk}^2\right). \quad (36)$$

After the integration, we have

$$\langle \psi_n | \psi_k \rangle = \frac{\pi^3}{(G_{11}G_{22} - G_{12}^2)^{3/2}}\, e^{-W}, \quad (37)$$

where

$$W \equiv S + G_{11}\lambda_1^2 + 2\,G_{12}\,(\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2) + G_{22}\lambda_2^2 +$$

$$+2\,(\boldsymbol{\lambda}_1, \mathbf{Y}_1) + 2\,(\boldsymbol{\lambda}_2, \mathbf{Y}_2), \quad (38)$$

$$\boldsymbol{\lambda}_1 \equiv \frac{G_{12}\mathbf{Y}_2 - G_{22}\mathbf{Y}_1}{G_{11}G_{22} - G_{12}^2}, \quad \boldsymbol{\lambda}_2 \equiv \frac{G_{12}\mathbf{Y}_1 - G_{11}\mathbf{Y}_2}{G_{11}G_{22} - G_{12}^2}.$$

In the case of basis (6), the matrix element for the kinetic energy of the center of mass of the system equals exactly zero. Thus, we need only to know the matrix elements for the kinetic energy of each of the three particles. For example, for the particle number $j = 3$, we have

$$\left\langle \psi_n \left| -\frac{\hbar^2}{2m_3}\triangle_3 \right| \psi_k \right\rangle =$$

$$= \int d\mathbf{r} d\boldsymbol{\rho}\; \psi_n^*(\mathbf{r}, \boldsymbol{\rho})\left(-\frac{\hbar^2}{2m_3}\triangle_3\right)\psi_k(\mathbf{r}, \boldsymbol{\rho}) \equiv$$

$$\equiv \frac{\hbar^2}{2m_3}\int d\mathbf{r} d\boldsymbol{\rho}\,(\nabla_{\boldsymbol{\rho}}\psi_n^*(\mathbf{r}, \boldsymbol{\rho}), \nabla_{\boldsymbol{\rho}}\psi_k(\mathbf{r}, \boldsymbol{\rho})) =$$

$$= \frac{4\hbar^2}{2m_3}\int d\mathbf{r} d\boldsymbol{\rho}\,(\alpha_n\boldsymbol{\rho} + \beta_n\mathbf{r} + \boldsymbol{\gamma}_n,\, \alpha_k\boldsymbol{\rho} + \beta_k\mathbf{r} + \boldsymbol{\gamma}_k) \times$$

$$\times\, e^{-\left(G_{11}\rho^2 + 2G_{12}(\boldsymbol{\rho},\mathbf{r}) + G_{22}r^2 + 2(\boldsymbol{\rho},\mathbf{Y}_1) + 2(\mathbf{r},\mathbf{Y}_2) + S\right)}, \quad (39)$$

where the function $\psi_k(\mathbf{r}, \boldsymbol{\rho})$ dependent on the Jacobi coordinates $\mathbf{r}$ and $\boldsymbol{\rho}$ should be understood as the function $\psi_k(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_3)$ from (6) with the arguments

$$\tilde{\mathbf{r}}_1 = -\frac{m_3}{M}\boldsymbol{\rho} - \frac{m_2}{m_1 + m_2}\mathbf{r},$$

$$\tilde{\mathbf{r}}_2 = -\frac{m_3}{M}\boldsymbol{\rho} + \frac{m_1}{m_1 + m_2}\mathbf{r}, \quad (40)$$

$$\tilde{\mathbf{r}}_3 = \frac{m_1 + m_2}{M}\boldsymbol{\rho},$$

and we used the denotations:

$$\alpha_n \equiv \left(\frac{m_3}{M}\right)^2(a_{1n} + a_{2n}) + \left(\frac{m_1 + m_2}{M}\right)^2 a_{3n},$$

$$\beta \equiv \frac{m_3\,(m_2 a_{1n} - m_1 a_{2n})}{M\,(m_1 + m_2)}, \quad (41)$$

$$\boldsymbol{\gamma}_n \equiv \frac{m_3}{M}\,(a_{1n}\mathbf{R}_{1n} + a_{2n}\mathbf{R}_{2n}) - \frac{m_1 + m_2}{M}a_{3n}\mathbf{R}_{3n}.$$

The rest denotations from (39) are given above in (36). After the integration in (39), we obtain, for this matrix element,

$$\left\langle \psi_n \left| -\frac{\hbar^2}{2m_3}\triangle_3 \right| \psi_k \right\rangle =$$

$$= \frac{2\hbar^2\pi^3}{m_3 U^{\frac{3}{2}}}\exp\left(-\left(S - \frac{Y_1^2}{G_{11}} - \frac{(G_{11}\mathbf{Y}_2 - G_{12}\mathbf{Y}_1)^2}{G_{11}U}\right)\right) \times$$

$$\times\left[\frac{3\alpha_n\alpha_k}{2G_{11}} + \left(\frac{3G_{11}}{2U} + \lambda_2^2\right)\nu_n\nu_k +\right.$$

$$+\left(\boldsymbol{\lambda}_2\,, \nu_n\boldsymbol{\gamma}_k + \nu_k\boldsymbol{\gamma}_n + \frac{2G_{12}\mathbf{Y}_1}{G_{11}^2} - (\alpha_n\beta_k + \alpha_k\beta_n)\frac{\mathbf{Y}_1}{G_{11}}\right) +$$

$$\left. +\left(\boldsymbol{\gamma}_n - \alpha_n\frac{\boldsymbol{Y}_1}{G_{11}}\,, \boldsymbol{\gamma}_k - \alpha_k\frac{\mathbf{Y}_1}{G_{11}}\right)\right], \quad (42)$$

where the most of denotations are given above, and where

$$U \equiv G_{11}G_{22} - G_{12}^2, \quad \nu_n \equiv \beta_n - \alpha_n\frac{G_{12}}{G_{11}}. \quad (43)$$

Instead of expression (13) for the matrix element of a component of the potential energy, we have

$$\left\langle \psi_n \middle| \exp\left(-b_s r_{12}^2\right) \middle| \psi_k \right\rangle = \int d\mathbf{r} d\boldsymbol{\rho}\, \psi^*(\mathbf{r},\boldsymbol{\rho})\, e^{-b_s r^2} \psi(\mathbf{r},\boldsymbol{\rho}) =$$

$$= \int d\mathbf{r} d\boldsymbol{\rho} e^{-\left(G_{11}\rho^2 + 2G_{12}(\boldsymbol{\rho},\mathbf{r}) + \tilde{G}_{22} r^2 + 2(\boldsymbol{\rho},\mathbf{Y}_1) + 2(\mathbf{r},\mathbf{Y}_2) + S\right)}, \quad (44)$$

where $\tilde{G}_{22} \equiv G_{22} + b_s$. Since expression (44) coincides with (35) regarding the substitution $G_{22} \to \tilde{G}_{22}$, the result of the integration in (44) will be the same as the right-hand side of (37), but with the substitution mentioned above in all the expressions, containing G_{22}.

Ultimately, we give the explicit expression for the Coulomb potential matrix element (compare with (32)):

$$\langle \psi_n | V_C(r_{12}) | \psi_k \rangle = Z_1 Z_2 e^2 \int d\mathbf{r} d\boldsymbol{\rho}\, \psi^*(\mathbf{r},\boldsymbol{\rho})\, \frac{1}{r}\, \psi(\mathbf{r},\boldsymbol{\rho}) =$$

$$= \frac{Z_1 Z_2 e^2 \pi^3 e^{-L}}{|\boldsymbol{\lambda}_2|\, U^{\frac{3}{2}}} \operatorname{erf}\left(|\boldsymbol{\lambda}_2| \sqrt{\frac{U}{G_{11}}} \right), \quad (45)$$

where

$$L \equiv S - \frac{Y_1^2}{G_{11}} - \frac{\lambda_2^2}{G_{11} U}. \quad (46)$$

When the wave function of the system is found (i.e., the variational parameters are chosen, and the coefficients C_k are determined from the solution of the algebraic system (7)), we can easily find the structure functions of the system (in particular, the density distributions, form factors, pair correlation functions, the momentum distributions, and others).

4. Preliminary Discussion of Convergence

To test the efficiency of the new basis, we consider a simple model of ^{12}C nucleus as the system of three α-particles with Hamiltonian (1), where $m_1 = m_2 = m_3 = m_\alpha = 3.7273794$ MeV/c^2 is the mass of an α-particle, $M = 3m_\alpha$ is the total mass of the system, and the pair potentials are identical for each pair of particles and consist of two terms,

$$V(r) = V_{\alpha\alpha}(r) + V_C(r), \quad (47)$$

where $V_{\alpha\alpha}(r)$ is an effective nuclear pairwise potential between α-particles, and $V_C(r) = 4e^2/r$ is the Coulomb repulsion between each pair of α-particles ($e^2 = 1.4399764$ MeV $\cdot$ fm). Since our purpose is only to test the convergence of the new proposed basis, we take the simplest version of the nuclear part $V(r_{nk})$ of the interaction between α-particles in the form of two Gaussian functions

$$V(r) = -V_1 \exp\left(-\left(\frac{r}{r_{01}}\right)^2 \right) + V_2 \exp\left(-\left(\frac{r}{r_{02}}\right)^2 \right), \quad (48)$$

where $V_1 = 223.44$ MeV, $V_2 = 500.0$ MeV, $r_{01} = 1.7$ fm, and $r_{02} = 1.25$ fm. This potential assumes the binding energy of the system of three α-particles to be 7.275 MeV (experimental value is 7.2748 MeV), and the charge radius of ^{12}C (in Helm approximation) to be 2.469 fm (experimental value is 2.4704 fm).

Omitting the detailed analysis of the convergence, we note that, using the traditional Gaussian basis [1, 2], we find the energy of the system to be 7.275 MeV (all the digits being reliable) with a few dozens of basic functions. At the same time, with the use of basis (3), we need hundreds functions to achieve the same accuracy. The reason is that the new basis contains functions which are not projected onto the state with a definite angular momentum (in our case of the ground state $L = 0$), while the functions of the Gaussian basis already prepared with zero angular momentum for the ground sate of the system. If one makes a projection of the basic functions (3) onto the state with a definite L, then the convergence of this basis would become competitive with the case of the Gaussian basis. But, an advantage of the new basis lies in the fact that we can omit a procedure of projection and consider all the possible states of the system in a universal (uniformed) way. The price of this universality of the basis is a somewhat more slow convergence of the method.

5. Conclusions

To summarize, we note that two versions of bases are proposed to be used in variational calculations of the bound states of an N-particle system with different angular momenta and permutational symmetries. Matrix elements are calculated in the explicit form for the kinetic energy operator and pairwise potentials (in the form of a superposition of Gaussian functions), as well as for the Coulomb interaction. A convergence of the variational procedure is briefly discussed using a model of ^{12}C nucleus as a system of three α-particles.

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1. Yu.A. Lashko, G.F. Filippov, V.S. Vasilevsky. Dynamics of two-cluster systems in phase space. *Nucl. Phys. A* **941**, 121 (2015).
2. O.M. Povoroznyk, V.S. Vasilevsky. Spectrum of resonance states in ^{6}He. Experimental and theoretical analyses. *Ukr. J. Phys.* **60**, No. 3, 201 (2015).
3. V.S. Vasilevsky, Yu.A. Lashko, G.F. Filippov. Two- and three-cluster decays of light nuclei within a hyperspherical harmonics approach. *Phys. Rev. C* **97**, 064605 (2018).
4. G.F. Filippov, I.P. Okhrimenko. On the possibility of using the oscillatory basis for solving continuous spectrum problems. *Sov. J. Nucl. Phys.* **32**, No. 4, 480 (1980).
5. G.F. Filippov. On the account of correct asymptotics in the expansions in the oscillatory basis. *Sov. J. Nucl. Phys.* **33**, No. 4, 488 (1981).
6. V.I. Kukulin, V.M. Krasnopol'sky. A stochastic variational method for few-body systems. *J. Phys. G Nucl. Phys.* **3**, No. 6, 795 (1977).
7. Y. Suzuki, K. Varga. *Stochastic Variational Approach to Quantum Mechanical Few-Body Problems* (Springer-Verlag, Berlin, Heidelberg, 1998) [ISBN: 978-3-540-65152-9].
8. B.E. Grinyuk, I.V. Simenog. Structure of the ^{6}He nucleus in the three-particle model. *Physics of Atomic Nuclei* **72**, No. 1, 6 (2009).
9. B.E. Grinyuk, I.V. Simenog. Three-particle structure of the halo nucleus ^{6}Li. *Nucl. Phys. Atomic Energy* **10**, No. 9, 9 (2009).
10. B.E. Grinyuk, M.V. Kuzmenko, I.V. Simenog. Precise study of the Efimov three-particle spectrum and structure functions within variational approach. *Ukr. J. Phys.* **48**, No. 10, 1014 (2003).
11. B.E. Grinyuk, D.V. Piatnytskyi, I.V. Simenog. Structure characteristics of a ^{4}He nucleus within the microscopic approach. *Ukr. J. Phys.* **52**, No. 5, 424 (2007).
12. B.E. Grinyuk, I.V. Simenog. Structure characteristics of light cluster nuclei with two extra nucleons. *Ukr. J. Phys.* **56**, No. 7, 635 (2011).
13. B.E. Grinyuk, I.V. Simenog. Structural properties of the ^{10}Be and ^{10}C four-cluster nuclei. *Physics of Atomic Nuclei* **77**, No. 4, 415 (2014).
14. B.E. Grinyuk, D.V. Piatnytskyi. Structure of ^{14}C and ^{14}O nuclei calculated in the variational approach. *Ukr. J. Phys.* **61**, No. 8, 674 (2016).
15. B.E. Grinyuk, D.V. Piatnytskyi. Structure of ^{14}N nucleus within a five-cluster model. *Ukr. J. Phys.* **62**, No. 10, 835 (2017).
16. B.E. Grinyuk, D.V. Piatnytskyi, V.S. Vasilevsky. The lowest excited states of ^{14}C and ^{14}O nuclei within a five-cluster model. *Nucl. Phys. A* **1030**, 122588 (2023).
17. A.G. Donchev, S.A. Kalachev, N.N. Kolesnikov, V.I. Tarasov. Carcass functions in variational calculations for few-body systems. *Physics of Atomic Nuclei* **67**, No. 12, 2154 (2004).

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УНІВЕРСАЛЬНИЙ КООРДИНАТНИЙ ГАУСОЇДНИЙ БАЗИС ДЛЯ РОЗРАХУНКУ ЗВ'ЯЗАНИХ СТАНІВ СИСТЕМ ДЕКІЛЬКОХ ЧАСТИНОК

Запропоновано новий простий базис для варіаційних розрахунків зв'язаних станів системи декількох частинок. Для системи N частинок із парними потенціалами взаємодії в явному вигляді отримано матричні елементи гамільтоніана системи. Розглянуто також модифікований базис, інваріантний відносно просторових трансляцій. Для прикладу розглянуто ядро ^{12}C як систему трьох α-частинок і коротко обговорено збіжність методу.

Ключові слова: система декількох частинок, варіаційний метод, варіаційний базис.