Some aspects related to the transformation of the three body wave function built on the Gaussian basis

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The three-body wave function built on the basis of the Gaussian function, calculated using the three-body Hamiltonian with the Pauli blocking operator is studied. As an example, the wave function of the ground state of the ^{9}Be was taken. Analytical expressions are presented for the overlap matrix elements of the basis function for both basic and alternative set of relative Jacobi coordinates. The correlation densities of the wave function are calculated and illustrated depending on the set of orbital quantum numbers.

Keywords: the three-body problem, Gaussian basis, relative Jacobi coordinates

Introduction

The three decades have passed since the significant large root mean square radii of the ^{6}He, ^{6}Li, ^{8}He, ^{8}Li, ^{9}Li, ^{9}Be exotic nuclei were revealed by Tanihata I. and co-workers [1]. Moreover, the nucleus ^{11}Li showed a remarkably large radius

suggesting a large deformation or a long tail in the matter distribution. These discoveries have allowed the existing science to look from a new perspective at the interaction of nucleons in atomic nuclei, and challenged already known theoretical methods. It is difficult to say, that there is a unified model describing all the observable characteristics of the exotic nuclei. Nevertheless, it is possible to single out a theoretical method that describe a sufficient number of observable properties of the being explored nuclei.

The essence of the Gaussian Expansion Method is in the expansion of the total wave function in terms of the Gaussian basis function. The solution of the Schrödinger equation for the few body problem is consisted in finding the factor, i.e. weight, of the matrix elements of the Hamiltonian calculated with the Gaussian functions, and, in varying the parameters of the arguments of the exponential function. It is interesting to note that this method is applicable for problems of $N = 2 - 7$ bodies [2]. The method has the advantage of expressing matrix elements in the analytical form, which one makes possible to do calculations quite quickly on ordinary desktop computers. It should also be noted that in this method the parameters of the wave function are varied in order to obtain the minimum eigenvalue of the Hamiltonian matrix. Therefore, the approach is also called as Stochastic Variational Method (SVM).

In the framework of this method a multicluster model [3] for halo nuclei were tested giving a unified description for the ground states of ^{6}He and ^{8}He in a model comprising an α-cluster and single-neutron clusters. The ^{6}He and ^{8}He energies are reproduced by the same effective force very well, and the matter radii obtained are similar to those of other sophisticated calculations.

By means of the SVM a model for three composite particles were successfully applied to study the ground state of the ^{6}Li nucleus making allowance for the Pauli principle [4, 5]. The model has been shown to permit a simultaneous description of the following observables of the ^{6}Li ground state: the binding energy, the rms charge radius, the αd spectroscopic factor, the asymptotic constant of the αd channel, the charge form factor, the magnetic elastic form factor, the spectrum of the low-lying states, the cigar shaped geometrical configuration, etc.

Due to the limited number of existing materials on this topic for practical application, the purpose of this work is to make the formulae for variational calculations accessible and open. The books in Ref. [6, 7, 8] have been mainly used to deduce equations. The obtained expressions are tested on the example of the ^{9}Be nucleus. In the first section, some vector re-coupling problems in quantum mechanics are given, an expression for the total three-body wave function and details of the transformation of the basis function from one set to other sets of Jacobi coordinates are given and analytical expressions for the overlap matrix elements, which can further be applied to the matrix elements of other quantum operators, are deduced. Results and discussions are given in the second section. The main conclusions are made in the last section.

1   Stochastic Variational Method

1.1   Some aspects from the quantum theory of angular momenta

A total angular momentum $\mathbf{j}$ are decomposed into two angular momenta $\mathbf{j}_1$ and $\mathbf{j}_2$ by means of the Clebsch-Gordan coefficient. For example, to quote a basis $|\,jm\rangle$ with the angular momentum j with its z-component m, the Clebsch-Gordan coefficient can be represented as follow

$$|\,jm\rangle = \sum_{m_1 m_2} \langle\, j_1 m_1\, j_2 m_2 \mid jm\, \rangle \mid j_1 m_1 \rangle \mid j_2 m_2 \rangle, \tag{1}$$

For non-zero values of the coefficient (1) vectors $\mathbf{j}_1$, $\mathbf{j}_2$ and $\mathbf{j}$ must satisfy the rule of triangle:

$$|j_1 - j_2| \le j \le j_1 + j_2$$
$$|j - j_2| \le j_1 \le j + j_2$$
$$|j_1 - j| \le j_2 \le j_1 + j$$

and the condition

$$m = m_1 + m_2.$$

If there are three vectors $\mathbf{j}_1, \mathbf{j}_2$ and $\mathbf{j}_3$, one can get a total angular momentum $\mathbf{j}$ in two ways

$$\mathbf{j} = (\mathbf{j_1} + \mathbf{j_2}) + \mathbf{j_3} = \mathbf{j_{12}} + \mathbf{j_3} \tag{2}$$
$$= \mathbf{j_1} + (\mathbf{j_2} + \mathbf{j_3}) = \mathbf{j_1} + \mathbf{j_{23}} \tag{3}$$

The Basis $|(j_1 j_2) j_{12}, j_3; jm\rangle$ and the basis $|j_1, (j_2 j_3);\ jm\rangle$ corresponding to Eq. (2) and Eq. (3) are related through a factor $U(\,j_1 j_2 j j_3;\ j_{12} j_{23})$, which is the Racah coefficient:

$$|(j_1 j_2) j_{12}, j_3; jm\rangle = \sum_{j_{23}} U(\,j_1 j_2 j j_3;\ j_{12} j_{23})\,|j_1, (j_2 j_3);\ jm\rangle. \tag{4}$$

Four angular momenta, $\mathbf{j_1}$, $\mathbf{j_2}$, $\mathbf{j_3}$ and $\mathbf{j_4}$, are added into the total momentum $\mathbf{j}$ by

$$\mathbf{j} = (\mathbf{j_1} + \mathbf{j_2}) + (\mathbf{j_3} + \mathbf{j_4}) = \mathbf{j_{12}} + \mathbf{j_{34}} \tag{5}$$
$$= (\mathbf{j_1} + \mathbf{j_3}) + (\mathbf{j_2} + \mathbf{j_4}) = \mathbf{j_{13}} + \mathbf{j_{24}} \tag{6}$$

Two basis $|\,j_1 j_2 (j_{12}),\ j_3 j_4 (j_{34});\ jm\rangle$ and $|\,j_1 j_3 (j_{13}),\ j_2 j_4 (j_{24});\ jm\rangle$, constructed respectively on the scheme Eq. 5 and Eq. 6, are related as follow

$$|\,j_1 j_2 (j_{12}),\ j_3 j_4 (j_{34});\ jm\rangle = \sum_{j_{13}, j_{24}} \begin{bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{bmatrix} |\,j_1 j_3 (j_{13}),\ j_2 j_4 (j_{24});\ jm\rangle \tag{7}$$

where transformation coefficient with square brackets is called a unitary 9j-symbol.

A spacial spherical harmonics is expressed like

$$\mathcal{Y}_{lm}(\mathbf{r}) = r^l Y_{lm}(\hat{r}) \tag{8}$$

where $Y_{lm}(\hat{r})$ – spherical function, which is a eigenfunction of angular part the $\Delta_{\hat{r}}$ Laplace operator. For $\mathbf{r} = a\mathbf{r}_1 + b\mathbf{r}_2$ a decomposition of the spacial spherical harmonics $\mathcal{Y}_{lm}(\mathbf{r})$ leads to the following equality

$$
\begin{aligned}
\mathcal{Y}_{lm}(\mathbf{r} = a\mathbf{r}_1 + b\mathbf{r}_2) &= \sum_{l_1,l_2,m_1,m_2} a^{l_1} b^{l_2} \langle\, l_1 m_1\; l_2 m_2 \mid lm\, \rangle \mathcal{D}(l,l_1,l_2) \times \\
&\quad \times \mathcal{Y}_{l_1 m_1}(\mathbf{r_1}) \mathcal{Y}_{l_2 m_2}(\mathbf{r_2}) \\
&= \sum_{l_1,l_2} a^{l_1} b^{l_2} \mathcal{D}(l,l_1,l_2) \left[\mathcal{Y}_{l_1}(\mathbf{r_1}) \times \mathcal{Y}_{l_2}(\mathbf{r_2}) \right]_{lm}
\end{aligned} \tag{9}
$$

with the condition $l = l_1 + l_2$, and $\mathcal{D}(l,l_1,l_2)$ is given by

$$\mathcal{D}(l,l_1,l_2) = \sqrt{\frac{4\pi(2l+1)!}{(2l_1+1)!(2l_2+1)!}} \tag{10}$$

Spherical harmonics with the argument are coupled as follow

$$\left[Y_{l_1}(\hat{r}) \times Y_{l_2}(\hat{r}) \right]_{lm} = \mathcal{C}(l_1,l_2,l) Y_{lm}(\hat{r}) \tag{11}$$

where the $\mathcal{C}(l_1,l_2,l)$ coefficient reads as

$$\mathcal{C}(l_1,l_2,l) = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \langle\, l_1 0\; l_2 0 \mid l0\, \rangle \tag{12}$$

It would be useful also note a coupling between two spherical hyper harmonics kind of

$$\left[Y_{l_{12}}^{(l_1 l_2)}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \times Y_{l_{34}}^{(l_3 l_4)}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \right]_{lm} = \sum_{l_{13} l_{24}} E_{l_{13} l_{24}}^{l_1 l_2 l_{12} l_2 l_4 l_{34} l} Y_{lm}^{(l_{13} l_{24})}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \tag{13}$$

where the coupling coefficient $E_{l_{13} l_{24}}^{l_1 l_2 l_{12} l_2 l_4 l_{34} l}$ is given as

$$E_{l_{13} l_{24}}^{l_1 l_2 l_{12} l_2 l_4 l_{34} l} = \begin{bmatrix} l_1 & l_2 & l_{12} \\ l_3 & l_4 & l_{34} \\ l_{13} & l_{24} & l \end{bmatrix} \mathcal{C}(l_1,l_3,l_{13}) \mathcal{C}(l_2,l_4,l_{24}). \tag{14}$$

1.2   The three-body wave function

As an example, in this work the $2\alpha - n$ three body model of the ^{9}Be nucleus is taken. The three-body wave function of the ^{9}Be nucleus with total spin J and spin projection M_J is represented as

$$\Psi^{JM_J} = \sum_i C_i \psi_i^{JM_J}(k, pq). \tag{15}$$

For simplicity the Jacobi coordinates $\mathbf{x}_k$ and $\mathbf{y}_k$ are down, the symbols k, p and q comply with the cluster indices (see Fig. 1), and the combination of indices

(k, pq) corresponds to a certain choice of Jacobi coordinates $\mathbf{x}_k$ and $\mathbf{y}_k$ of the three-body system, where $\mathbf{x}_k$ is a vector of the relative distance between the pair of particles pq and k, and $\mathbf{y}_k$ is the vector of the relative distance between the center of mass of the pair pq and the particle k. The coefficients C_i in Eq. (ref totwf) are the parameters of the wave function expansion and are found as a result of solving the generalized eigenvalue problem.

The explicit form of the basis functions $\psi_i^\gamma(k, pq)$ is chosen in the form of the multiplication of the spatial and spin wave functions:

$$\psi_i^{JM_J}(k, pq) = \left[\phi_i^\gamma(k, pq) \times \chi^S\right]_{JM_J},$$ (16)

here the index γ includes the quantum numbers $L\lambda l$. The spatial part $\phi_i^\gamma(k, pq)$ of the wave function (16) is constructed using the Gaussian functions:

$$\phi_i^\gamma(k, pq) = x_k^\lambda y_k^l exp\left(-\tfrac{1}{2}\alpha_i^{(k)}x_k^2 - \tfrac{1}{2}\beta_i^{(k)}y_k^2\right)[Y_\lambda(\hat{\mathbf{x}}_k) \times Y_l(\hat{\mathbf{y}}_k)]_{LM_L},$$ (17)

where L and M_L are the total orbital momentum of the system and its projection, λ, l are the orbital moments conjugated to the coordinates $\mathbf{x}_k$ and $\mathbf{y}_k$ respectively, $\alpha_i^{(k)}$, $\beta_i^{(k)}$ are the linear parameters of the three-body wave function.

1.3 Transformation of the basis function

The chosen form of the basis function (16) is convenient in that it can be easily transformed for use with an alternative set of Jacobi coordinates. A rotation matrix connecting different sets of the Jacobi coordinates is provided through

$$\begin{pmatrix}\mathbf{x}_k \\ \mathbf{y}_k\end{pmatrix} = \mathbf{T}^{(kq)}\begin{pmatrix}\mathbf{x}_q \\ \mathbf{y}_q\end{pmatrix}.$$ (18)

here, particularly for the (kq) transition, the $\mathbf{T}^{(kq)}$ matrix is

$$\mathbf{T}^{(kp)} = \begin{pmatrix}\mathbf{T}_{11}^{(kq)} & \mathbf{T}_{12}^{(kq)} \\ \mathbf{T}_{21}^{(kq)} & \mathbf{T}_{22}^{(kq)}\end{pmatrix} = \begin{pmatrix}-\frac{m_p}{m_p+m_q} & 1 \\ -\frac{m_q(m_k+m_p+m_q)}{(m_p+m_q)(m_k+m_q)} & -\frac{m_k}{(m_k+m_q)}.\end{pmatrix}$$ (19)

There is no need to consider the transformation of spin part of the basis function. The reason is that the S spin of the $2\alpha - n$ three-body system is defined only by the vacant nucleon, and it doesn't depend on the choice of the
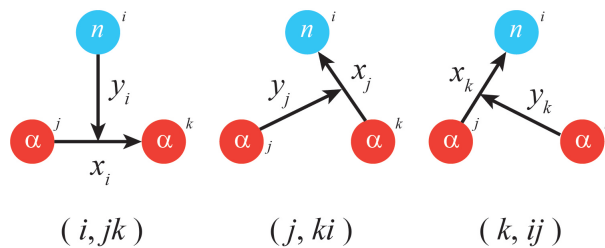

Figure 1: The schemes of the three-body system on the example of ^{9} Be.

Jacobi coordinate. That is to say, the coupling of the vacant nucleon spin with the $\alpha - \alpha$ subsystem spin gives again the spin of the nucleon due to the boson statistics of α particles.

The transformation of the space part of the wave function from the set (k, qp) to the set (q, kp) can be expressed in the following way

$$\phi_i^\gamma (k, pq) = \sum_{\tilde\gamma} A_{\tilde\gamma\gamma} \left(\mathbf{T}^{(kq)} \right) \phi_i^{\tilde\gamma} (q, kp), \tag{20}$$

where the sum is over quantum numbers of the $\tilde\gamma$ new set, and the new basis function is

$$\phi_i^{\tilde\gamma} (q, kp) = x_q^{\tilde\lambda} y_q^{\tilde l} exp \left(-\tfrac{1}{2}\alpha_i^{(q)} x_q^2 - \tfrac{1}{2}\beta_i^{(q)} y_q^2 - \rho_i^{(q)} \mathbf{x}_q \cdot \mathbf{y}_q \right) \times$$
$$\times \left[Y_{\tilde\lambda} \left(\hat{\mathbf{x}}_q \right) \times Y_{\tilde l} \left(\hat{\mathbf{y}}_q \right) \right]_{LM_L}, \tag{21}$$

where new parameters of the wave function are given by

$$\begin{pmatrix} \alpha_i^{(q)} & \rho_i^{(q)} \\ \rho_i^{(q)} & \beta_i^{(q)} \end{pmatrix} = \left(\mathbf{T}^{(kq)} \right)^T \times \begin{pmatrix} \alpha_i^{(k)} & \rho_i^{(k)} \\ \rho_i^{(k)} & \beta_i^{(k)} \end{pmatrix} \times \mathbf{T}^{(kq)}. \tag{22}$$

Note, that for the (k, pq) coordinate set the radial wave function (17) does not include the scalar product $\mathbf{x}_k \cdot \mathbf{y}_k$, which means $\rho_i^{(k)} = 0$. Using Eq. (9) and (13) it is easy to get the coupling coefficient $A_{\tilde\gamma\gamma} \left(\mathbf{T}^{(kq)} \right)$ from Eq. (20), which is defined as follow

$$A_{\tilde\gamma\gamma} \left(\mathbf{T}^{(kq)} \right) = \sum_{\lambda_1 \lambda_2 l_1 l_2} \left(\mathbf{T}_{11}^{(kq)} \right)^{\lambda_1} \left(\mathbf{T}_{12}^{(kq)} \right)^{\lambda_2} \left(\mathbf{T}_{21}^{(kq)} \right)^{l_1} \left(\mathbf{T}_{22}^{(kq)} \right)^{l_2} \times$$
$$\times E_{\tilde\lambda\tilde l}^{\lambda_1\lambda_2\lambda l_1 l_2 lL} \mathcal{D}(\lambda, \lambda_1, \lambda_2) \mathcal{D}(l, l_1, l_2). \tag{23}$$

1.4   Overlap matrix elements

Within the (k, pq) scheme an overlap matrix element, in particular for the space part $\phi_i^\gamma (k, pq)$ of the basis function, is expressed by

$$\langle \phi_i^\gamma (k, pq) | \phi_j^{\gamma'} (k, pq) \rangle = \int \int d\mathbf{x}_k d\mathbf{y}_k \, \phi_i^\gamma (k, pq) \left(\phi_j^{\gamma'} (k, pq) \right)^*. \tag{24}$$

Following the properties of spherical harmonics the latter six dimensional integral gets $\delta_{\gamma\gamma'}$. Then, it is reduced to analytical expression as

$$\mathcal{I} \left(\lambda, l, \alpha_{ij}^{(k)}, \beta_{ij}^{(k)} \right) = 2^{1+\lambda+l} \frac{\Gamma \left(\tfrac{3}{2} + \lambda \right) \Gamma \left(\tfrac{3}{2} + l \right)}{\left(\alpha_{ij}^{(k)} \right)^{\frac{3}{2}+\lambda} \left(\beta_{ij}^{(k)} \right)^{\frac{3}{2}+l}}. \tag{25}$$

with

$$\alpha_{ij}^{(k)} = \alpha_i^{(k)} + \alpha_j^{(k)} \qquad \beta_{ij}^{(k)} = \beta_i^{(k)} + \beta_j^{(k)} \tag{26}$$

However, to calculate overlap matrix elements for arbitrary basis functions, for example

$$\langle \phi_i^{\tilde\gamma} (q, kp) | \phi_j^{\tilde\gamma'} (q, kp) \rangle = \int \int d\mathbf{x}_k d\mathbf{y}_k \, \phi_i^{\tilde\gamma} (q, kp) \left(\phi_j^{\tilde\gamma'} (q, kp) \right)^*, \tag{27}$$

one must handle with the scalar product $exp\left(-\rho\mathbf{x}\cdot\mathbf{y}\right)$ in Eq. (21), in which radial and angular parts are mixed. It makes a problem in integration procedure, consequently, mathematical techniques must be applied. There are two tricks to solve this problem. First is the solution of problem is in expansion of the exponential function into the partial waves. Another one is in projection of the factor of scalar product into the rotation matrix $\mathbf{T}$. Both approaches give the same results in calculation of the matrix elements.

1.4.1 By means of the exponential function expansion

The expansion of exponential function is given by

$$exp(-\rho\mathbf{x}\cdot\mathbf{y}) = 4\pi\sum_{\kappa}\sqrt{2\kappa+1}\epsilon(\kappa,\rho)i_{\kappa}(|\rho|xy)Y_{00}^{(\kappa\kappa)}(\hat{\mathbf{x}},\hat{\mathbf{y}}) \tag{28}$$

where $i_{\kappa}(x)$ – modified spherical Bessel function of the first kind, $\epsilon(\kappa,\rho) = (-1)^{\kappa}$ for $\rho\leq0$, otherwise it equals to 1. Once radial part is separated, defining an integral

$$\int_{0}^{\infty}\int_{0}^{\infty}dxdy\ x^{2\lambda+\kappa+2}y^{2l+\kappa+2}exp\left(-\alpha x^2-\beta y^2\right)i_{\kappa}(|\rho|xy), \tag{29}$$

one can get its analytical form

$$\mathcal{I}(\lambda,l,n,\alpha,\beta,|\rho|) = \sqrt{\frac{\pi}{8}}(2l)!!\ \Gamma(l+n+\tfrac{3}{2})\ |\rho|^n\ \beta^{-l-n-\frac{3}{2}}\times$$

$$\times\sum_{\kappa=0}^{l}\frac{\Gamma(\kappa+\lambda+n+\tfrac{3}{2})}{\kappa!(l-\kappa)!\Gamma(\kappa+n+\tfrac{3}{2})}\left(\frac{\rho^2}{2\beta}\right)^{\kappa}\left(\frac{\alpha}{2}-\frac{\rho^2}{2\beta}\right)^{-\kappa-\lambda-n-\frac{3}{2}}. \tag{30}$$

The angular part is integrated all over angular variables, then, it can be expressed analytically in the following way

$$\int\int d\hat{\mathbf{x}}\ d\hat{\mathbf{y}}\ Y_{00}^{(\kappa\kappa)}(\hat{\mathbf{x}},\hat{\mathbf{y}})Y_{L'M_{L'}}^{(\lambda'l')}(\hat{\mathbf{x}},\hat{\mathbf{y}})\left(Y_{LM_L}^{(\lambda l)}(\hat{\mathbf{x}},\hat{\mathbf{y}})\right)^{*} = E_{\lambda l}^{\kappa\kappa0\lambda'l'LL}\delta_{LL'} \tag{31}$$

Using the property of the 9-j symbol, in which one of the numbers is zero, $E_{\lambda l}^{\kappa\kappa0\lambda'l'LL}$ can be reduced as

$$E_{\lambda l}^{\kappa\kappa0\lambda'l'LL} = U\left(\lambda L\kappa l';l\lambda'\right)\frac{\mathcal{C}\left(\lambda',\lambda,\kappa\right)\mathcal{C}\left(l',l,\kappa\right)}{\sqrt{(2L+1)\left(2\kappa+1\right)}}. \tag{32}$$

The Jacobian matrix $\mathbf{J}^{(kq)}$ for transformation from the $\mathbf{x}_k,\mathbf{y}_k$ coordinates to the $\mathbf{x}_q,\mathbf{y}_q$ coordinates gives the $\mathbf{T}^{(kq)}$ matrix

$$\mathbf{J}^{(kq)} = \begin{pmatrix}\frac{\partial\mathbf{x}_k\left(\mathbf{x}_q,\mathbf{y}_q\right)}{\partial\mathbf{x}_q} & \frac{\partial\mathbf{x}_k\left(\mathbf{x}_q,\mathbf{y}_q\right)}{\partial\mathbf{y}_q} \\ \frac{\partial\mathbf{y}_k\left(\mathbf{x}_q,\mathbf{y}_q\right)}{\partial\mathbf{x}_q} & \frac{\partial\mathbf{y}_k\left(\mathbf{x}_q,\mathbf{y}_q\right)}{\partial\mathbf{y}_q}\end{pmatrix} = \mathbf{T}^{(kq)}. \tag{33}$$

Accordingly, the determinant $|\mathbf{J}^{(kq)}|$ is a determinant of the $\mathbf{T}^{(kq)}$ matrix, which equals to 1:

$$|\mathbf{J}^{(kq)}| = |\mathbf{T}^{(kq)}| = 1 \tag{34}$$

Therefore, the integration variables in Eq. (27) can be changed without any factorization.

Lastly, an expression for the overlap matrix element of the (q, kp) coordinate sets (27) can be determined as follow

$$\langle \phi_i^{\tilde{\gamma}}(q, kp) | \phi_j^{\tilde{\gamma}'}(q, kp) \rangle = \int \int d\mathbf{x}_k d\mathbf{y}_k \, \phi_i^{\tilde{\gamma}}(q, kp) \left(\phi_j^{\tilde{\gamma}'}(q, kp) \right)^* =$$

$$= 4\pi \sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}} \left(T^{(kq)} \right) A_{\gamma\tilde{\gamma}'} \left(T^{(kq)} \right) \sum_{\kappa} \sqrt{2\kappa + 1} \, \epsilon(\kappa, \rho) E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL} \times$$

$$\times \mathcal{I} \left(\tfrac{\tilde{\lambda}+\tilde{\lambda}'-\kappa}{2}, \tfrac{\tilde{l}+\tilde{l}'-\kappa}{2}, \kappa, \alpha_{ij}^{(q)}, \beta_{ij}^{(q)}, |\rho_{ij}^{(q)}| \right). \tag{35}$$

with $\rho_{ij}^{(q)} = \rho_i^{(q)} + \rho_j^{(q)}$.

1.4.2 By means of the projection into the $\mathbf{T}$ matrix

In this approach the rotation matrix $\mathbf{Q}$, projecting the scalar product in the radial part of the wave function, is implemented by

$$\mathbf{Q}_i^{(kq)} = \mathbf{T}^{(kq)} \times \begin{pmatrix} 1 & -\frac{\rho_i^{(q)}}{\alpha_i^{(q)}} \\ 0 & 1 \end{pmatrix}. \tag{36}$$

Consequently, the radial part of the wave function can be rewritten with no scalar product term as

$$\phi_i^{\tilde{\gamma}}(q, kp) = x_q^{\tilde{\lambda}} y_q^{\tilde{l}} exp \left(-\tfrac{1}{2}\alpha_i^{(q)} x_q^2 - \tfrac{1}{2} \left(\beta_i^{(q)} - \tfrac{\left(\rho_i^{(q)}\right)^2}{\alpha_i^{(q)}} \right) y_q^2 \right) \times$$

$$\times \left[Y_{\tilde{\lambda}}(\hat{\mathbf{x}}_q) \times Y_{\tilde{l}}(\hat{\mathbf{y}}_q) \right]_{LM_L}. \tag{37}$$

One can get easily the expression of the overlap matrix element for the (q, kp) coordinate sets (27) can be determined as follow

$$\langle \phi_i^{\tilde{\gamma}}(q, kp) | \phi_j^{\tilde{\gamma}'}(q, kp) \rangle = \int \int d\mathbf{x}_k d\mathbf{y}_k \, \phi_i^{\tilde{\gamma}}(q, kp) \left(\phi_j^{\tilde{\gamma}'}(q, kp) \right)^* =$$

$$= \sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}} \left(\mathbf{Q}_{ij}^{(kq)} \right) A_{\gamma\tilde{\gamma}'} \left(\mathbf{Q}_{ij}^{(kq)} \right) \mathcal{I} \left(\tilde{\lambda}, \tilde{l}, \alpha_{ij}^{(q)}, \left(\beta_{ij}^{(q)} - \tfrac{\left(\rho_{ij}^{(q)}\right)^2}{\alpha_{ij}^{(q)}} \right) \right) \delta_{\tilde{\gamma}\tilde{\gamma}'}. \tag{38}$$

Analogously, changing the integration variables is carried out with no factorizations due to the $|\mathbf{Q}_i^{(kq)}| = 1$. Notably, rotation matrix becomes depended on the ij indexes in this approach.

1.5 Normalization and correlation density of the three-body wave function

Using the overlap matrix elements the normalization of the total three-body wave function is given by

$$\mathcal{N}^{(k)} = \langle \Psi^{JM_J} | \Psi^{JM_J} \rangle = \sum_{\gamma} \mathcal{N}_{\gamma}^{(k)},$$

$$\mathcal{N}_{\gamma}^{(k)} = \sum_{ij} C_i C_j \mathcal{I}\left(\lambda, l, \alpha_{ij}^{(k)}, \beta_{ij}^{(k)}\right). \tag{39}$$

For the alternative set of Jacobi coordinates the overlap of the total wave function is given by

$$\mathcal{N}^{(q)} = \langle \Psi^{JM_J} | \Psi^{JM_J} \rangle = \sum_{\gamma} \sum_{\gamma'} \mathcal{N}_{\gamma\gamma'}^{(q)} \tag{40}$$

It should be mentioned, that in the latter expression the basis functions is not orthogonal. Therefore, according to the Eq. (31) the sum is limited with the condition $\delta_{LL'}$ only. Using the analytical form of overlap matrix element (30), $\mathcal{N}_{\gamma\gamma'}^{(q)}$ can be given by

$$\mathcal{N}_{\gamma\gamma'}^{(q)} = 4\pi \sum_{ij} C_i C_j \sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}}\left(\mathbf{T}^{(kq)}\right) A_{\gamma\tilde{\gamma}'}\left(\mathbf{T}^{(kq)}\right) \times$$

$$\times \sum_{\kappa} \sqrt{2\kappa+1}\, \epsilon(\kappa, \rho_{ij}^{(k)}) E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL} \times$$

$$\times \mathcal{I}\left(\tfrac{\tilde{\lambda}+\tilde{\lambda}'-\kappa}{2}, \tfrac{\tilde{l}+\tilde{l}'-\kappa}{2}, \kappa, \alpha_{ij}^{(q)}, \beta_{ij}^{(q)}, |\rho_{ij}^{(q)}|\right), \tag{41}$$

or using the Eq. (38)

$$\mathcal{N}_{\gamma\gamma'}^{(q)} = \sum_{ij} C_i C_j \sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}}\left(\mathbf{Q}_{ij}^{(kq)}\right) A_{\gamma\tilde{\gamma}'}\left(\mathbf{Q}_{ij}^{(kq)}\right) \times$$

$$\times \mathcal{I}\left(\tilde{\lambda}, \tilde{l}, \alpha_{ij}^{(q)}, \left(\beta_{ij}^{(q)} - \frac{\left(\rho_{ij}^{(q)}\right)^2}{\alpha_{ij}^{(q)}}\right)\right) \delta_{\tilde{\gamma}\tilde{\gamma}'}. \tag{42}$$

A correlation density function of the total wave function (15) can be expressed in the following way

$$W(x_k, y_k) = \sum_{\gamma} W_{\gamma}(x_k, y_k)$$

$$W_{\gamma}(x_k, y_k) = \sum_{ij} C_i C_j x_k^{2+2\lambda} y_k^{2+2l} exp\left(-\tfrac{1}{2}\alpha_{ij}^{(k)} x_k^2 - \tfrac{1}{2}\beta_{ij}^{(k)} y_k^2\right). \tag{43}$$

Results and discussions

The numerical values of the coefficients C_i, $\alpha_i^{(k)}$ and $\beta_i^{(k)}$ for the ground state of the ^{9}Be nucleus have been taken from Ref. [9]. In this work, calculation

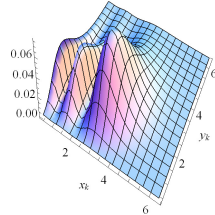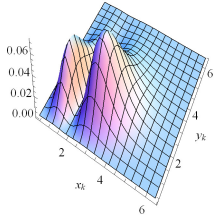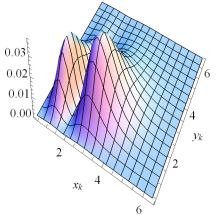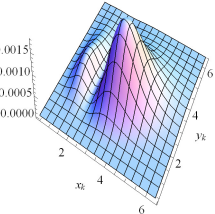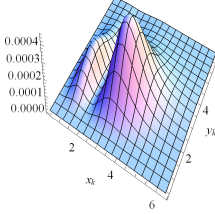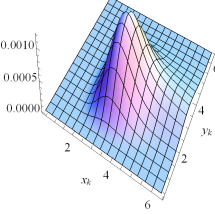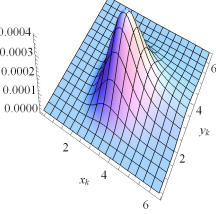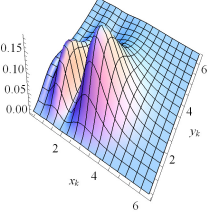|	$\gamma \equiv \lambda l L$			
	011	211	212	231
$\mathcal{N}_\gamma^{(k)}$	0.4358	0.3619	0.1826	0.0091
$\mathcal{N}_{\gamma\gamma}^{(q)}$	0.4358	0.3619	0.1826	0.0091
$W_\gamma(x_k, y_k)$				

	$\gamma \equiv \lambda l L$			
	232	431	432	$\sum_i \gamma_i$
$\mathcal{N}_\gamma^{(k)}$	0.0022	0.0064	0.0019	1.0
$\mathcal{N}_{\gamma\gamma}^{(q)}$	0.0022	0.0064	0.0019	1.0
$W_\gamma(x_k, y_k)$				

Table 1: Values of the $\mathcal{N}_\gamma^{(k)}$ and $\mathcal{N}_{\gamma\gamma}^{(q)}$ normalizations for each γ's, and 3-d plot of the correlation density function $W_\gamma(x_k, y_k)$ of the wave function depending on γ.
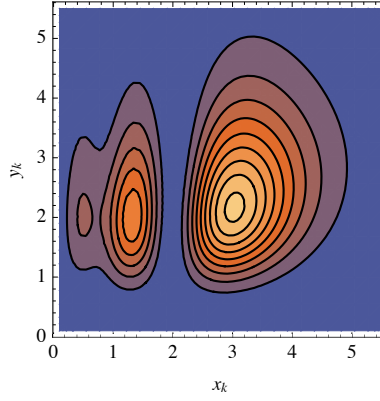
Figure 2: The contour plot of the correlation density function $W(x_k, y_k)$.

of the three-body wave function has been carried out within the framework of the variational method, solving the Hill-Wheeler integral equations using the three-dimensional Schrödinger equation for the three particle nuclear system. The $\alpha\alpha$-interaction is the deep attractive potential with the Pauli-forbidden states, parametrized in the Gaussian function form. The αn-potential is also attractive with the Pauli projection only for S-state, and it has different deep depending on parity of l-momentum (for more details, see [10, 9]).

The $\mathcal{N}_\gamma^{(k)}$ normalization of the total wave function for each γ's are listed in Tab. 1. It has no physical reasons to calculate the normalization $\mathcal{N}^{(q)}$ in the (q, kp) scheme. However, for verification of expressed above equations it would be useful to show their correctness. For this purpose the $\mathcal{N}_{\gamma\gamma'}^{(q)}$ normalization was calculated with the condition $\delta_{\gamma\gamma'}$. The calculated results for the $\mathcal{N}_{\gamma\gamma}^{(q)}$ are listed in Tab. 1. Comparison of the $\mathcal{N}_\gamma^{(k)}$ with $\mathcal{N}_{\gamma\gamma}^{(q)}$, calculated for overlap matrix elements by means of the both approaches shown in the Sec. 1.4.1 and 1.4.2, is showing the same values as in Ref. [9]. That means correctness of all above deduced equations.

New basis functions are summed over all the new $\tilde{\lambda}$ and $\tilde{l}$ orbital moments with the condition $\lambda + l = \tilde{\lambda} + \tilde{l}$. It is valid only in case of $L \leq \lambda + l$. However, during the calculations it was revealed, that in the $L < \lambda + l$ case, the condition $\lambda + l = \tilde{\lambda} + \tilde{l}$ does not perform equality in Eq. (20). For example, lets take the $\phi_i^\gamma(k, pq)$ basis function with $\gamma_2 \equiv 211$ ($\lambda = 2$, $l = 1$, and $L = 1$). Transforming it into the $\phi_i^{\tilde{\gamma}}(q, kp)$ new basis function, the new basis function is summed not only over the $\tilde{\gamma} \equiv 211$ or 211, it must be also summed over 011, 101 quantum numbers. Moreover, in case of $\lambda + l > L$ the $x_q^{\tilde{\lambda}} y_q^{\tilde{l}}$ factor must be putted away from Eq. (21) and placed in Eq. (23). The transformation coefficient now depends on x_q and y_q as

$$A_{\tilde{\gamma}\gamma}\left(\mathbf{T}^{(kq)}\right) = \sum_{\lambda_1\lambda_2 l_1 l_2} x_q^{\lambda_1+l_1} y_q^{\lambda_2+l_2} \left(\mathbf{T}_{11}^{(kq)}\right)^{\lambda_1} \left(\mathbf{T}_{12}^{(kq)}\right)^{\lambda_2} \left(\mathbf{T}_{21}^{(kq)}\right)^{l_1} \left(\mathbf{T}_{22}^{(kq)}\right)^{l_2} \times$$
$$\times E_{\tilde{\lambda}\tilde{l}}^{\lambda_1\lambda_2\lambda l_1 l_2 lL} \mathcal{D}(\lambda, \lambda_1, \lambda_2) \mathcal{D}(l, l_1, l_2).$$

After these and summing level changes the Eq. (20) turns to right equality.

The correlation density functions $W_\gamma(x_k, y_k)$ for each γ are plotted and presented in Tab. 1. In each partial correlation density exact peaks are seen. The reason of this is in the nature of $\alpha\alpha$ and αn interactions. They keep the Pauli principle. The case, when the both potentials implement the Pauli projector, is $\gamma_1 \equiv 011$, which has three peaks. It was mentioned above, that αn-potential has fordidden S-state. In the other cases, for $\lambda + l = 3$ and $\lambda + l = 5$, only the $\alpha\alpha$ interaction keeps the Pauli principle – there are only two peaks.

It is interesting to demonstrate a contour plot of the correlation density function $W(x_k, y_k)$ in Fig.2. Three different structural configurations are mainly manifested with the (x_k, y_k) coordinate positions: $(0.5, 2.0)$ $(1.2, 2.0)$ and $(3.0, 2.0)$. It worth to draw attention, that all the three configurations are in the same y_k coordinate. The similar geometrical configuration were found also for the ^{6}Li and ^{6}He nuclei in Ref. [5].

Conclusion

In the framework of the SVM the three body wave function based on the Gaussian functions was studied. Deduced overlap matrix elements of the basis on the basic and alternative set of the Jacobi coordinates were obtained by means of two approaches. It was found that, in case of $\lambda + l > L$, the condition $\lambda + l = \tilde{\lambda} + \tilde{l}$ given in Ref. [6] becomes not correct. Addition quantum numbers should be summed in order to keep the equality between the (k, pq) and (q, kp) basis functions following the $|\lambda - l| \leq \tilde{\lambda} \leq \lambda + l$ and $|\lambda - l| \leq \tilde{l} \leq \lambda + l$ conditions. Obtained analytical equations can be useful for a calculating other matrix elements.

On the example of the ^{9}Be nucleus the weights of γ components and correlation density function for each γ's were listed in the table. The same results of the normalizations within the both approaches were obtained in comparing with the values in Ref. [9], what means correctness of the deduced expressions.

The contour plot was demonstrated of the ground state wave function of the ^{9}Be nucleus. Coordinates of the three main geometrical configurations were extracted. Such kind of structure plays important role in nuclear transfer reactions and will useful for the DWBA calculations.

References

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