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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. Analytical expressions are presented for the matrix elements of the overlap of the basis functions 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 numbers also for the both sets of Jacobi coordinates.

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

Introduction

N years have passed since the skin, halo effects of such exotic nuclei were shown by Tanihata. These discoveries have allowed the existing science to look from a new perspective at the interactions 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 the observable properties of the being explored nuclei.

It is Gaussian Expansion Method. The essence is in the expansion of the total wave function in terms of the Gaussian basis function. The solution of the Schroedinger equation for the few body problem is reduced to finding the factor, i.e. weight, of the matrix elements of the Hamiltonian calculated through the exponential functions, to set the parameters of the arguments of the exponential function. It is interesting to note that this method is easily applicable for problems of two bodies, three bodies and four bodies. 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.

Due to the limited number of existing materials on this topic for practical application, the purpose of this work is to make the formulas for variational calculations accessible and open. In the first section, some vector re-coupling problems in quantum mechanics are given, an expression for the total three-particle wave function and details of the transformation of the basis function from one set to other sets of Jacobi coordinates are given. Then, the second section deduces analytical expressions for the overlap matrix elements, which can further be applied to the matrix elements of other quantum operators. The main conclusions are made in the conclusion section.

1 Theoretical model

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 $\mid jm\rangle$ with the angular momentum $\mathbf{j}$ with its z-component m, the Clebsch-Gordan coefficient can be represented as follow

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

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

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

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

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

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

$$\mathcal{C}(l_1,l_2,l)=\sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}}\langle\, l_10\; l_20 \mid l0\,\rangle \tag{12}$$

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

$$\left[Y_{l_{12}}^{(l_1l_2)}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\times Y_{l_{34}}^{(l_3l_4)}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\right]_{lm}=\sum_{l_{13}l_{24}}E_{l_{13}l_{24}}^{l_1l_2l_{12}l_2l_4l_{34}l}Y_{lm}^{(l_{13}l_{24})}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) \tag{13}$$

where the coupling coefficient $E_{l_{13}l_{24}}^{l_1l_2l_{12}l_2l_4l_{34}l}$ is given as

$$E_{l_{13}l_{24}}^{l_1l_2l_{12}l_2l_4l_{34}l}=\begin{bmatrix} l_1 & l_2 & l_{12}\\ l_3 & l_4 & l_{34}\\ l_{13} & l_{24} & l\end{bmatrix}\mathcal{C}(l_1,l_3,l_{13})\mathcal{C}(l_2,l_4,l_{24}). \tag{14}$$

1.2 The three-body wave function

The three-body wave function with total spin J and spin projection M_J is represented as

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

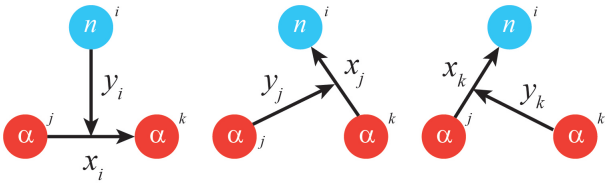
For simplicity the Jacobi coordinates $\mathbf{x}_k$ and $\mathbf{y}_k$ are down, the symbols k, p and q comply with the cluster indices (see Fig. 1), and the combination of indices $(k,\ pq)$ corresponds to a certain choice of Jacobi coordinates $\mathbf{x}_k$ and $\mathbf{y}_k$ of the three-body system, 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:

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

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:

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



(i, jk) (j, ki) (k, ij)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

one must handle with the scalar product $exp(-\rho\mathbf{x}\cdot\mathbf{y})$ 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 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 $\rho \leq 0$, 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

$$\mathcal{I}(\lambda, l, n, \alpha, \beta, |\rho|) = \sqrt{\frac{\pi}{8}}(2l)!!\,\Gamma(l+n+\tfrac{3}{2})\,|\rho|^n\,\beta^{-l-n-\frac{3}{2}}\times$$
$$\times\sum_{\kappa=0}^{l}\frac{\Gamma(\kappa+\lambda+n+\frac{3}{2})}{\kappa!(l-\kappa)!\Gamma(\kappa+n+\frac{3}{2})}\left(\frac{\rho^2}{2\beta}\right)^{\kappa}\left(\frac{\alpha}{2}-\frac{\rho^2}{2\beta}\right)^{-\kappa-\lambda-n-\frac{3}{2}}. \tag{30}$$

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

$$\int\int d\hat{\mathbf{x}}\, d\hat{\mathbf{y}}\; Y_{00}^{(\kappa\kappa)}(\hat{\mathbf{x}},\hat{\mathbf{y}}) Y_{L'M_{L'}}^{(\lambda' l')}(\hat{\mathbf{x}},\hat{\mathbf{y}}) \left(Y_{LM_L}^{(\lambda l)}(\hat{\mathbf{x}},\hat{\mathbf{y}})\right)^* = E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL}\delta_{LL'} \tag{31}$$

Using the property of the 9-j symbol, in which one of the numbers is zero, $E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL}$ can be reduced as

$$E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL} = U\left(\lambda L\kappa l';\, l\lambda'\right) \frac{\mathcal{C}\left(\lambda',\lambda,\kappa\right)\mathcal{C}\left(l',l,\kappa\right)}{\sqrt{\left(2L+1\right)\left(2\kappa+1\right)}}. \tag{32}$$

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

$$\begin{aligned} \int\int d\mathbf{x}_k d\mathbf{y}_k\; \phi_i^{\tilde{\gamma}}\left(q,kp\right)\left(\phi_j^{\tilde{\gamma}'}\left(q,kp\right)\right)^* = \\ = 4\pi \sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}}\left(T^{(kq)}\right) A_{\gamma\tilde{\gamma}'}\left(T^{(kq)}\right) \sum_{\kappa} \sqrt{2\kappa+1}\, \epsilon(\kappa,\rho) E_{\lambda l}^{\kappa\kappa 0\lambda' l' LL} \times \\ \times \mathcal{I}\left(\tfrac{\tilde{\lambda}+\tilde{\lambda}'-\kappa}{2},\ \tfrac{\tilde{l}+\tilde{l}'-\kappa}{2},\ \kappa,\ \alpha_{ij}^{(q)},\ \beta_{ij}^{(q)},\ |\rho_{ij}^{(q)}|\ \right). \end{aligned} \tag{35}$$

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

1.4.2 By means of the projection into the 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

$$\begin{aligned} \phi_i^{\tilde{\gamma}}\left(q,kp\right) = & x_q^{\tilde{\lambda}} y_q^{\tilde{l}} exp\left(-\tfrac{1}{2}\alpha_i^{(q)} x_q^2 - \tfrac{1}{2}\left(\beta_i^{(q)} - \frac{\left(\rho_i^{(q)}\right)^2}{\alpha_i^{(q)}}\right) y_q^2\right) \times \\ & \times \left[Y_{\tilde{\lambda}}\left(\hat{\mathbf{x}}_q\right) \times Y_{\tilde{l}}\left(\hat{\mathbf{y}}_q\right)\right]_{LM_L}. \end{aligned} \tag{37}$$

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

$$\int\int d\mathbf{x}_k d\mathbf{y}_k\, \phi_i^{\tilde{\gamma}}(q,kp)\left(\phi_j^{\tilde{\gamma}'}(q,kp)\right)^* = \\ =\sum_{\tilde{\gamma}\tilde{\gamma}'} A_{\gamma\tilde{\gamma}}\left(\mathbf{Q}_{ij}^{(kq)}\right) A_{\gamma\tilde{\gamma}'}\left(\mathbf{Q}_{ij}^{(kq)}\right)\mathcal{I}\left(\tilde{\lambda},\tilde{l},\alpha_{ij}^{(q)},\left(\beta_{ij}^{(q)}-\frac{\left(\rho_{ij}^{(q)}\right)^2}{\alpha_{ij}^{(q)}}\right)\right)\delta_{\tilde{\gamma}\tilde{\gamma}'}. \tag{38}$$

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

$$\mathcal{N}^{(k)} =\langle\Psi^{JM_J}|\Psi^{JM_J}\rangle=\sum_{\gamma}\mathcal{N}_{\gamma}^{(k)}, \\ \mathcal{N}_{\gamma}^{(k)} =\sum_{ij}C_iC_j\mathcal{I}\left(\lambda,l,\alpha_{ij}^{(k)},\beta_{ij}^{(k)}\right). \tag{39}$$

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

$$\mathcal{N}_{\gamma\gamma'}^{(q)} =4\pi\sum_{ij}C_iC_j\sum_{\tilde{\gamma}\tilde{\gamma}'}A_{\gamma\tilde{\gamma}}\left(\mathbf{T}^{(kq)}\right)A_{\gamma\tilde{\gamma}'}\left(\mathbf{T}^{(kq)}\right)\times \\ \times\sum_{\kappa}\sqrt{2\kappa+1}\,\epsilon(\kappa,\rho_{ij}^{(k)})E_{\lambda l}^{\kappa\kappa0\lambda'l'LL}\times \\ \times\mathcal{I}\left(\tfrac{\tilde{\lambda}+\tilde{\lambda}'-\kappa}{2},\ \tfrac{\tilde{l}+\tilde{l}'-\kappa}{2},\ \kappa,\ \alpha_{ij}^{(q)},\ \beta_{ij}^{(q)},\ |\rho_{ij}^{(q)}|\ \right), \tag{41}$$

or using the Eq. (38)

$$\mathcal{N}_{\gamma\gamma'}^{(q)} =\sum_{ij}C_iC_j\sum_{\tilde{\gamma}\tilde{\gamma}'}A_{\gamma\tilde{\gamma}}\left(\mathbf{Q}_{ij}^{(kq)}\right)A_{\gamma\tilde{\gamma}'}\left(\mathbf{Q}_{ij}^{(kq)}\right)\times \\ \times\mathcal{I}\left(\tilde{\lambda},\tilde{l},\alpha_{ij}^{(q)},\left(\beta_{ij}^{(q)}-\frac{\left(\rho_{ij}^{(q)}\right)^2}{\alpha_{ij}^{(q)}}\right)\right)\delta_{\tilde{\gamma}\tilde{\gamma}'}. \tag{42}$$

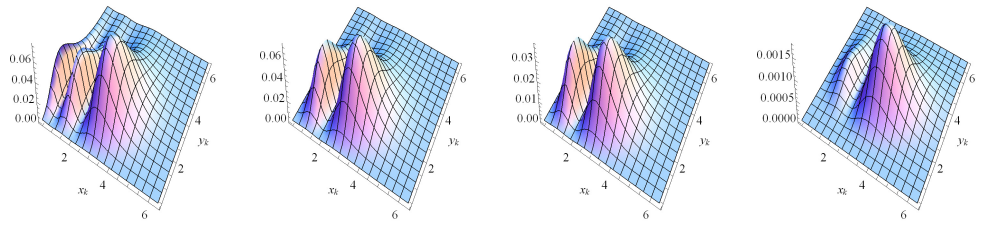
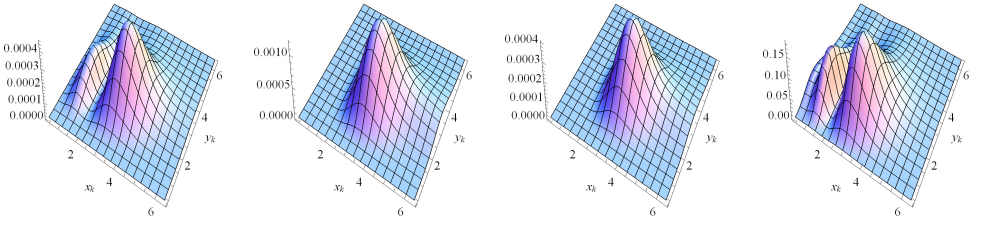
	$\gamma \equiv \lambda IL$			
	011	211	212	231
$\mathcal{N}_{\gamma}^{(k)}$	0.4358	0.3619	0.1826	0.0091
$\mathcal{N}_{\gamma\gamma}^{(q)}$	0.4358	0.3619	0.1826	0.0091
$W_{\gamma}(x_k, y_k)$				
	$\gamma \equiv \lambda IL$			
	232	431	432	$\sum_i \gamma_i$
$\mathcal{N}_{\gamma}^{(k)}$	0.0022	0.0064	0.0019	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.

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

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

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 [Kukulin]. In this work, calculation 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 Schrodinger 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.

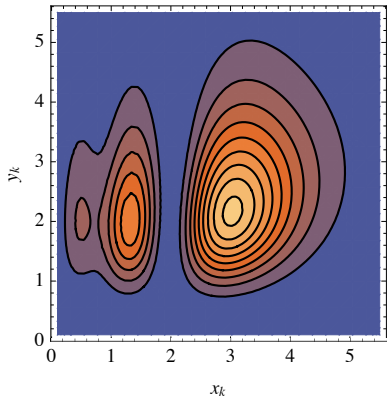


Figure 2: The counter plot of the correlation density function $W(x_k, y_k)$.

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. [Kukulin]. 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 $L > \lambda + l$. 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

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

After these little 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 three configuration are in the same y_k coordinate. The first configuration is due to the nature of the αn-potential. Such kind of structure of the ground state of the ^{9}Be nucleus has significant importance in the transfer reaction calculation.

Conclusion

Your Conclusion text comes here...

Acknowledgments

Also, use this section to provide information about funding by including specific grant numbers and titles. If you need to include funding information, list the name(s) of the funding organization(s) in full, and identify which authors received funding for what.

References

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[1] Bass R, Nuclear Reactions with Heavy IonsBerlin (Heidelberg, New York: Springer-Verlag, 1980) 410 p.(DOI or ISBN)

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[2] Tanihata I. et al., Phys.Lett.B. **206** (1988) 592-600.(DOI)

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[3] Oganessian Y.Ts., Proceeding of the International Conference on Nuclear Physics, Munich **73** (1975) 351-360.(DOI)

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[3] Oganessian Y.Ts., Proceeding of the International Conference on Nuclear Physics, Munich **73** (1975) 351-360.(DOI)