

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

B.A. Urazbekov^{1,2,3,4}, A.S. Denikin^{2,3}, N. Itaco^{1,4}, N.T. Tusunbayev³

¹Dipartimento di Matematica e Fisica, Università degli Studi della Campania "Luigi Vanvitelli", Caserta, Italy

²Dubna state university, Dubna, Russia

³Joint institute for nuclear research, Dubna, Russia

⁴Istituto Nazionale di Fisica Nucleare, Complesso Univeristario di Monte S. Angelo, Napoli, Italy

e-mail: bakytzhan.urazbekov@gmail.com

DOI: 10.29317/***** entered by Editors

Received: **, ** - after revision

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

$$|jm\rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | jm \rangle |j_1 m_1\rangle |j_2 m_2\rangle, \quad (1)$$

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

$$\begin{aligned} |j_1 - j_2| &\leq j \leq j_1 + j_2 \\ |j - j_2| &\leq j_1 \leq j + j_2 \\ |j_1 - j| &\leq j_2 \leq j_1 + j \end{aligned}$$

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

$$\mathbf{j} = (\mathbf{j}_1 + \mathbf{j}_2) + \mathbf{j}_3 = \mathbf{j}_{12} + \mathbf{j}_3 \quad (2)$$

$$= \mathbf{j}_1 + (\mathbf{j}_2 + \mathbf{j}_3) = \mathbf{j}_1 + \mathbf{j}_{23} \quad (3)$$

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 $U(j_1 j_2 j_3; j_{12} j_{23})$, which is the Racah coefficient:

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

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

$$\mathbf{j} = (\mathbf{j}_1 + \mathbf{j}_2) + (\mathbf{j}_3 + \mathbf{j}_4) = \mathbf{j}_{12} + \mathbf{j}_{34} \quad (5)$$

$$= (\mathbf{j}_1 + \mathbf{j}_3) + (\mathbf{j}_2 + \mathbf{j}_4) = \mathbf{j}_{13} + \mathbf{j}_{24} \quad (6)$$

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

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

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

A spacial spherical harmonics is expressed like

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

where $Y_{lm}(\hat{r})$ – spherical function, which is a eigenfunction of angular part the Δ 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

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

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

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

Spherical harmonics with the argument are coupled as follow

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

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

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

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

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

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

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

1.2 The three-body wave function

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

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

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.

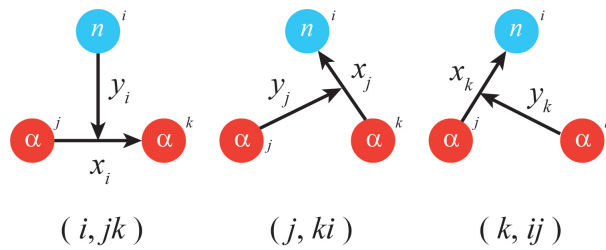


Figure 1: The schemes of the three-body system on the example of ^9Be .

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:

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

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:

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

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

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

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

$$\phi_i^\gamma(k, pq) = \sum_{\tilde{\gamma}} A_{\tilde{\gamma}\gamma}^{(kq)} \phi_i^{\tilde{\gamma}}(q, kp), \quad (19)$$

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

$$\begin{aligned} \phi_i^{\tilde{\gamma}}(q, kp) = & x_q^{\tilde{\lambda}} y_q^{\tilde{l}} \exp \left(-\alpha_i^{(q)} x_q^2 - \beta_i^{(q)} y_q^2 - 2\rho_i^{(q)} \mathbf{x}_q \cdot \mathbf{y}_q \right) \times \\ & \times [Y_{\tilde{\lambda}}(\hat{\mathbf{x}}_q) \times Y_{\tilde{l}}(\hat{\mathbf{y}}_q)]_{LM_L}, \end{aligned} \quad (20)$$

where new parameters of the wave function are

$$\begin{aligned} \alpha_i^{(q)} &= \alpha_i^{(k)} T_{11}^2 + \beta_i^{(k)} T_{21}^2 \\ \beta_i^{(q)} &= \alpha_i^{(k)} T_{12}^2 + \beta_i^{(k)} T_{22}^2 \\ \rho_i^{(q)} &= 2\alpha_i^{(k)} T_{11} T_{12} + 2\beta_i^{(k)} T_{21} T_{22} \end{aligned} \quad (21)$$

Using Eq. (9) and (13) it is easy to get the coupling coefficient $A_{\tilde{\gamma}\gamma}^{(kq)}$ from Eq. (19), which is defined as follow

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

1.4 Overlap matrix elements

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

$$\begin{aligned} \mathcal{I}(\gamma, i, j) &= \int \int d\mathbf{x}_k d\mathbf{y}_k \phi_i^\gamma(k, pq) \left(\phi_j^{\gamma'}(k, pq) \right)^* \\ &= C_i C_j \frac{\Gamma(\frac{3}{2} + \lambda) \Gamma(\frac{3}{2} + l)}{4(\alpha_i + \alpha_j)^{\frac{3}{2} + \lambda} (\beta_i + \beta_j)^{\frac{3}{2} + l}} \delta_{\gamma\gamma'}. \end{aligned} \quad (23)$$

However, to calculate overlap matrix elements for arbitrary basis functions, one must handle with the scalar product $\exp(-\rho \mathbf{x} \cdot \mathbf{y})$ in Eq. (20), 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, the solution of problem is in expansion of the exponential function into the partial waves; another one, in projection of the factor of scalar product into the rotation matrix. Both approach 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

$$\exp(-\rho \mathbf{x} \cdot \mathbf{y}) = 4\pi \sum_{\kappa} \sqrt{2\kappa + 1} \epsilon(\kappa, \rho) i_{\kappa}(|\rho|xy) Y_{00}^{(\kappa\kappa)}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \quad (24)$$

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

$$\int_0^{\infty} \int_0^{\infty} dx dy x^{2\lambda+\kappa+2} y^{2l+\kappa+2} \exp(-\alpha x^2 - \beta y^2) i_{\kappa}(|\rho|xy), \quad (25)$$

one can get its analytical form

$$\begin{aligned} \mathcal{I}(\lambda, l, n, \alpha, \beta, |\rho|) = & \sqrt{\frac{\pi}{8}} (2l)!! \Gamma(l + n + \frac{3}{2}) |\rho|^n \beta^{-l-n-\frac{3}{2}} \times \\ & \times \sum_{\kappa=0}^l \frac{\Gamma(\kappa + \lambda + n + \frac{3}{2})}{\kappa!(l - \kappa)! \Gamma(\kappa + n + \frac{3}{2})} \left(\frac{\rho^2}{2\beta}\right)^{\kappa} \left(\frac{\alpha}{2} - \frac{\rho^2}{2\beta}\right)^{-\kappa-\lambda-n-\frac{3}{2}}. \end{aligned} \quad (26)$$

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

$$\int \int d\hat{\mathbf{x}} d\hat{\mathbf{y}} Y_{00}^{(\kappa\kappa)}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) Y_{LM_L}^{(\lambda'l')}(\hat{\mathbf{x}}, \hat{\mathbf{y}}) \left(Y_{LM_L}^{(\lambda l)}(\hat{\mathbf{x}}, \hat{\mathbf{y}})\right)^* = E_{\lambda l}^{\kappa\kappa 0 \lambda' l' LL}. \quad (27)$$

Results and discussions

The calculation of the three-body wave function was carried out within the framework of the variational method for solving the Hill-Wheeler integral equations obtained on the basis of the three-dimensional Schrodinger equation for a three-part nuclear system, which is described in detail in cite kukulin1984detailed. The numerical values of the coefficients were calculated by us earlier and for the ground state of the ${}^9\text{Be}$ nucleus are given in the work cite voronchev1994analysis.

2 Aidos notations

The energy dependence of total cross sections of reactions ${}^6\text{He} + \text{Si}$ and ${}^6,{}^9\text{Li} + \text{Si}$ in the beam energy range 5-30 MeV/nucleon has been measured. An agreement with the published experimental data for the reaction ${}^6\text{He} + \text{Si}$ was obtained. For the reaction ${}^9\text{Li} + \text{Si}$ new data in the vicinity a local enhancement of the total cross section was obtained. Theoretical analysis of possible reasons of appearance of this peculiarity in the collisions of nuclei ${}^6\text{He}$ and ${}^9\text{Li}$ with Si nuclei has been carried out including the influence of external neutrons of weakly bound projectile nuclei.

Table 1.

Please write your table caption here (*the width of the table should be equal to the width of the text*)

H	q	α_q	$\chi^2/d.o.f.$	Confidence level of fittings
0.3	2	0.56 ± 0.01	0.38	98.90 %
	3	1.22 ± 0.03	0.49	95.93 %
	4	1.92 ± 0.06	0.58	91.30 %
	5	2.63 ± 0.10	0.70	80.95 %
1	2	0.59 ± 0.01	0.74	76.62 %

Construct	Benefits	Drawbacks
Option	Straightforward	Don't get error reason
Try	Returns error reason	Requires exception
Or	Returns error reason	Third-party library
Either	Returns error reason	Works by convention

Table 1: The pros and cons of Scala's optional classes

Example of text style and formula design in the text

In our experiments, we employed the Dubna gas-filled recoil separator (DGRFS), that allows the separation of the products of complete fusion reactions from the beam of bombarding ions, elastically-scattered nuclei, and products of incomplete fusion. The detection system includes proportional chambers used to measure the time of flight (TOF) of particles and several semiconductor detectors with position-sensitive strips.

The principle of operation of the separator is selection of products of the complete-fusion reaction by their charge state q in a rare gas and kinematic characteristics (mass of recoil nucleus m and its velocity v) in accordance with the separator magnetic rigidity $B\rho = mv/q$ (note, q depends linearly on v). These values are calculated for the xn -reaction channel when setting the

separator's parameters.

The DGFRS strongly separates forward-peaked evaporation residues (ER), products of complete-fusion reactions, within a narrow angle with a huge suppression of the products of the transfer reactions and even incomplete fusion, e.g., αxn reactions. The TOF selection in the existing separators may be complemented and reinforced by the combined measurement of recoil energy and TOF. Note, the production properties "separator", "mass separation", "angular selection", and "TOF selection" were called "assignment properties" in [3].

Subsection title

Formulas should be written follow type:

$$TC(HKL) = \frac{I(hkl)}{I_0(hkl)} \bigg/ \frac{1}{n} \sum \frac{I(hkl)}{I_0(hkl)}, \quad (28)$$

Example of figure style

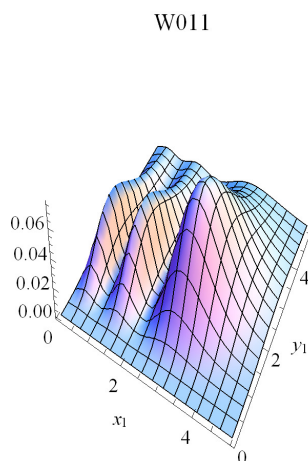


Figure 1. Please write your figure caption here.

The first superheavy nucleus ^{289}Fl was discovered in the $^{244}\text{Pu}(^{48}\text{Ca}, 3n)$ reaction studied at DGFRS (here and after we refer to reviews [1,2] containing references to most of earlier experimental data). The decay properties of ^{289}Fl and descendant nuclei are shown in figure 1.

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

For books: Author, *Book title* (Publisher, place year) page numbers.(DOI or ISBN)

Example:

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

For articles from journals: Author, Journal **Volume** (year) page numbers.(DOI)

Example:

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

For conference materials, proceedings, etc.: Author, Publication title: Type of publication **Volume** (year) page numbers.(DOI) Example:

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

Example:

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

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

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