

# Some aspects related to 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.

## Theoretical model

### Some aspects from the quantum theory of angular moments

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. ?? and Eq. ??, 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.

## The three-body wave function

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. In this approach, the total wave function with total spin  $J$  and spin projection  $M_J$  is represented as

$$\Psi_{JM_J} = \sum_i C_i^{(i)} \phi_i^\gamma(i, jk) \quad (8)$$

here, for simplicity of further presentation, the spatial Jacobi coordinates  $\mathbf{x}_i$  and  $\mathbf{y}_i$  are omitted, the symbols  $i, j, k$  correspond to the cluster indices (see Fig. 1), and the combination of indices  $(i, jk)$  corresponds to a certain choice of Jacobi coordinates  $\mathbf{x}_i$  and  $\mathbf{y}_i$  of the considered three-body system, where  $\mathbf{x}_i$  is a vector the relative distance between the pair of particles  $j$  and  $k$ , and  $\mathbf{y}_i$  is the vector of the relative distance between the center of mass of the pair  $j$  and  $k$  and the particle  $i$ . The coefficients  $C_i^{(i)}$  in the expression ( ref totwf) are the parameters of the wave function expansion and are found as a result of solving the variational problem. 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.

The explicit form of the basis functions  $\phi_l^\gamma(i, jk)$  is chosen in the form of the direct product of the spatial and spin wave functions:

$$\phi_l^\gamma(i, jk) = [\Phi_l^\gamma(i, jk) \otimes \chi_s]_{JM_I} \quad (9)$$

here the index  $\gamma$  includes the quantum numbers  $L\lambda l$ . The spatial part  $\Phi_l^\gamma(i, jk)$  of the wave function (ref subwf) is constructed using the multidimensional Gaussian functions:

$$\Phi_l^\gamma(i, jk) = x_i^\lambda y_i^l \exp\left(-\alpha_i^{(i)} x_i^2 - \beta_i^{(i)} y_i^2\right) [Y_\lambda(\hat{x}_i) \otimes Y_l(\hat{y}_i)]_{LM_L} \quad (10)$$

where  $L$  and  $M_L$  are the total orbital momentum of the system and its projection,  $\lambda, l$  are the orbital moments conjugate to the coordinates  $\mathbf{x}_i$  and  $\mathbf{y}_i$  respectively,  $\alpha_i^{(i)}, \beta_i^{(i)}$  are the parameters of the wave function, the values of which are given in the work cite voronchev1994analysis.

The chosen form of the basis functions is convenient in that it can be easily transformed for use with an alternative set of Jacobi coordinates. In particular, the transformation of the spatial part of the wave function from the set  $(i, jk)$  to the set  $(j, ki)$  can be expressed in the following form

$$\Phi_l^\gamma(i, jk) = \sum_{\tilde{\gamma}} A_{\tilde{\gamma}\gamma}^{j \leftarrow i} \Phi_l^{\tilde{\gamma}}(j, ki) \quad (11)$$

where the sum is over the quantum numbers of the set  $\tilde{\gamma}$ , taking into account the condition  $\tilde{\lambda} + \tilde{l} = \lambda + l$ . The reconnection factors  $A_{\tilde{\gamma}\gamma}^{j \leftarrow i}$  are defined as follows cite suzuki1998stochastic

$$A_{\tilde{\gamma}\gamma}^{j \leftarrow i} = (-1)^{\lambda+l} \sum_{\lambda_1 \lambda_2 l_1 l_2} \left( \Omega_{11}^{j \leftarrow i} \right)^{\lambda_1} \left( \Omega_{12}^{j \leftarrow i} \right)^{\lambda_2} \left( \Omega_{21}^{j \leftarrow i} \right)^{l_1} \left( \Omega_{22}^{j \leftarrow i} \right)^{l_2} \times \quad (12)$$

$$\sqrt{\frac{[\lambda]![l]![\lambda][l][\lambda_1][l_1][\lambda_2][l_2][\tilde{\lambda}][\tilde{l}]}{[\lambda_1]![l_1]![\lambda_2]![l_2]!}} \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \lambda_1 & \lambda_2 & \lambda \\ l_1 & l_2 & l \\ \tilde{\lambda} & \tilde{l} & L \end{pmatrix},$$

where  $[x] = 2x + 1$ , matrices with dimensions  $2 \times 3$  and  $3 \times 3$  are  $3j$  and  $9j$  Wigner coefficients, respectively, and the elements of the matrix  $\Omega_{nm}^{j \leftarrow i}$  are defined as follows

$$\Omega^{j \leftarrow i} = \frac{1}{\sqrt{(m_j + m_k)(m_i + m_k)}} \begin{pmatrix} -\sqrt{m_i m_j} & -\sqrt{m_k M} \\ \sqrt{m_k M} & \sqrt{m_i m_j} \end{pmatrix}$$

here the value  $M = m_i + m_j + m_k$ .

## Overlap matrix elements

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

### 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.,  $\alpha xn$  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:

$$TC(HKL) = \frac{I(hkl)}{I_0(hkl)} \bigg/ \frac{1}{n} \sum \frac{I(hkl)}{I_0(hkl)}, \quad (13)$$

## Example of figure style

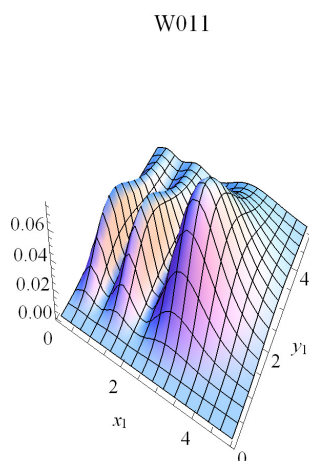


Figure 1. Please write your figure caption here.

The first superheavy nucleus  $^{289}\text{Fl}$  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  $^{289}\text{Fl}$  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)