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VARIATIONAL APPROACH TO THE COULOMB THREE-BODY BOUND STATE PROBLEM

It is known that the variational methods are the most powerful tool for studying the Coulomb three-body bound state problem. In this work the exponential explicitly correlated variational basis set of the type $\exp(-\alpha_s r_1 - \beta_s r_2 - \gamma_s r_{12})$ with complex exponents is considered. It will be shown that the method yields the best bound state energies for many known atomic and molecular systems.

1. Introduction. Variational methods for numerical calculation of the Coulomb bound state problem were developed by many authors [1]–[6] since the very beginning of the Quantum Mechanics. The first simple explicitly correlated basis set were introduced in 1928 by Hylleraas [1, 2]:

$$\psi(r_1, r_2) = e^{-\frac{1}{2}t} \sum c_{lmn} s^l u^m t^n, \quad (1)$$

$$s = r_1 + r_2, u = r_{12}, t = r_2 - r_1,$$

where r_1 and r_2 are the position vectors of two electrons with respect to a nucleus.

Later it became clear that at least for the atomic helium ground state it is essential to incorporate into the expansion logarithmic terms of the type $\ln \rho$,

where $\rho = (r_1^2 + r_2^2)^{1/2}$. This kind of the wave function behaviour at small ρ was predicted analytically by Bartlett and Fock [7]. In 1966, Frankowski and Pekeris introduced the compact representation [3] of the form

$$\psi(r_1, r_2) = e^{-kt} \sum c_{lmn} s^l u^m t^{2m} \times (s^2 + t^2)^{j/2} (\ln)^j, \quad (2)$$

Inclusion of the logarithmic term into the variational wave function brought substantial improvement of nonrelativistic energies for the two electron atoms.

With advance of computer power, basis sets became simplified that allowed for calculating numerous matrix elements required for relativistic and QED corrections. Further efforts were concentrated on a choice of strategy to generate the most efficient and flexible basis sets within the same form of basis functions. In [4] the double basis set with generalized Hylleraas trial function

$$\psi(r_1, r_2) = \sum C_{ijk}^A r_1^i r_2^j r_{12}^k e^{-\alpha_s r_1 - \beta_s r_2} + \sum C_{ijk}^B r_1^i r_2^j r_{12}^k e^{-\alpha_s r_1 - \beta_s r_2} \quad (3)$$

were used. This double basis set technique along with full optimization of nonlinear parameters at each basis set yield substantial progress in accuracy. However, further advance is hindered by the numerical instability even in quadruple precision arithmetic due to almost linear dependence of the basis set at large N .

The method of our work is further continuation of these latter ideas.

2. Variational expansion. Expansion we want to explore here is very similar to the generalized Hylleraas basis set, but instead of using the polynomials over Hylleraas variables we generate nonlinear parameters in the exponents in a quasi-random manner. This method has been successfully used in calculations [5, 6] previously. Obviously, the matrix elements can be evaluated in the same way as for the generalized Hylleraas basis set (3). In our approach we are using complex exponents. It is easily seen that if one replaces real exponents by complex ones the analytical integrals will remain exactly the same.

The variational wave function is expanded in a form

$$\psi_0 = \sum_{i=0}^{N/2} \left\{ U_i \operatorname{Re} \left[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} \right] + W_i \operatorname{Im} \left[e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_{12}} \right] \right\} Y_{l_1 l_2}^{LM}(r_1, r_2) \quad (4)$$

Here α_i , β_i , and γ_i are complex parameters generated in a quasi-random way [8, 9]:

$$\alpha_i = \left[\frac{1}{2} i(i+1) \sqrt{p_a} \right] (A_2 - A_1) + A_1 + \left\{ \left[\frac{1}{2} i(i+1) \sqrt{q_a} \right] (A'_2 - A'_1) + A'_1 \right\}, \quad (5)$$

$[x]$ designates the fractional part of x , p_α and q_α are some prime numbers, $[A_1, A_2]$ and $[A'_1, A'_2]$ are real variational intervals which need to be optimized. Parameters β_i and γ_i are obtained in a similar way. Functions in Eq. (4) are the solid bipolar harmonics

$$Y_{l_1 l_2}^{LM}(r_1, r_2) = r_1^{l_1} r_2^{l_2} \{Y_{l_1} \otimes Y_{l_2}\}_{LM},$$

An important feature of the method is that it demonstrates a very fast convergence. The general rule which can be inferred experimentally from the use of the method is that increasing of the basis by about 200 functions yields about one additional digit in the variational energy for large basis sets of $N \sim 2000$. The minor deficiency is that the basis quickly degenerates when N increases. Already for moderate $N \sim 250-400$ a quadruple precision is required.

Using this method we want to solve the bound state problem for a system of three particles interacting via Coulomb forces. The nonrelativistic Hamiltonian for such a system may be written:

$$H = -\frac{1}{2\mu_1} \nabla_1^2 - \frac{1}{2\mu_2} \nabla_2^2 - \frac{1}{m_3} \nabla_3^2 + \frac{Z_1 Z_3}{r_1} + \frac{Z_2 Z_3}{r_2} + \frac{Z_1 Z_2}{r_{12}}, \quad (6)$$

where μ_1 and μ_2 are the reduced masses of particles 1 and 2 with respect to a third particle, Z_1 , Z_2 and Z_3 are arbitrary charges of three particles.

3. Evaluation of the Hamiltonian. It is convenient to write down explicitly the action of the gradient operators on the trial functions:

$$\begin{aligned} \nabla_1 [Y_{l_1 l_2}^{l_1 l_2}(r_1, r_2) F(r_1, r_2, r_{12})] = \\ = [\nabla_1 Y_{l_1 l_2}^{l_1 l_2}] F(\cdot) + Y_{l_1 l_2}^{l_1 l_2} \left\{ \left[\frac{r_1}{r_1} \frac{\partial}{\partial r_1} + \frac{r_1 - r_2}{r_{12}} \right] F(\cdot) \right\}, \quad (7) \end{aligned}$$

Then by using the conventional angular momentum algebra [10] one may find how the operators appearing in the Hamiltonian (6) acts on the regular bipolar harmonics:

$$\begin{aligned} \nabla_1^2 Y_{l_1 l_2}^{l_1 l_2}(r_1, r_2) = \nabla_2^2 Y_{l_1 l_2}^{l_1 l_2}(r_1, r_2) = 0, \\ (\nabla_1 \cdot \nabla_2) Y_{l_1 l_2}^{l_1 l_2}(r_1, r_2) = \\ = C(l_1, l_2) Y_{l_1 l_2}^{l_1 l_2-1}(r_1, r_2), \quad (8a) \end{aligned}$$

Where

$$\begin{aligned} C(l_1, l_2) = C(l_2, l_1) = (-1)^{l_1+l_2+L} (2l_1+1)(2l_2+1) \times \\ \times \sqrt{l_1 l_2} \begin{Bmatrix} l_1 & l_2 & L \\ l_2-1 & l_1-1 & 1 \end{Bmatrix}. \end{aligned}$$

The next set of operators, which are required, are

$$\begin{aligned} (r_1 \cdot \nabla_1) Y_{l_1 l_2}^{l_1 l_2} = l_1 Y_{l_1 l_2}^{l_1 l_2}, \\ (\nabla_1 \cdot r_2) Y_{l_1 l_2}^{l_1 l_2} = A(l_1, l_2) Y_{l_1 l_2}^{l_1-1, l_2+1} + \\ + B(l_1, l_2) r_2^2 Y_{l_1 l_2}^{l_1-1, l_2-1}, \quad (8b) \end{aligned}$$

Where

$$\begin{aligned} A(l_1, l_2) = -(-1)^{l_1+l_2+L} (2l_1+1) \times \\ \times \sqrt{l_1(l_2+1)} \begin{Bmatrix} l_1 & l_2 & L \\ l_2+1 & l_1-1 & 1 \end{Bmatrix}, \\ B(l_1, l_2) = \frac{C(l_1, l_2)}{(2l_2+1)}. \end{aligned}$$

With the use of the above expressions one may find formulas for the kinetic energy operator. For brevity of notation we use $\partial_i = 1/r_i \cdot (\partial/\partial r_i)$, then

$$\begin{aligned} \nabla_1^2 Y_{l_1 l_2}^{l_1 l_2} F(r_1, r_2, r_{12}) = 2[\nabla_1 Y_{l_1 l_2}^{l_1 l_2}] \nabla_1 F + \\ + Y_{l_1 l_2}^{l_1 l_2} \nabla_1^2 F = 2[l_1 Y_{l_1 l_2}^{l_1 l_2} (\partial_1 + \partial_{12}) - A(l_1, l_2) \\ \times Y_{l_1 l_2}^{l_1-1, l_2+1} \partial_{12} - B(l_1, l_2) Y_{l_1 l_2}^{l_1-1, l_2-1} r_2^2 \partial_{12}] F \\ + Y_{l_1 l_2}^{l_1 l_2} \nabla_1^2 F, \quad (9a) \end{aligned}$$

and

$$\begin{aligned} (\nabla_1 \cdot \nabla_2) Y_{l_1 l_2}^{l_1 l_2} F(r_1, r_2, r_{12}) = [(\nabla_1 \cdot \nabla_2) Y_{l_1 l_2}^{l_1 l_2}] F \\ + [\nabla_1 Y_{l_1 l_2}^{l_1 l_2}] \nabla_2 F + [\nabla_2 Y_{l_1 l_2}^{l_1 l_2}] \nabla_1 F \\ + Y_{l_1 l_2}^{l_1 l_2} (\nabla_1 \cdot \nabla_2) F = \{A(l_1, l_2) Y_{l_1 l_2}^{l_1+1, l_2-1} \\ \times (\partial_1 + \partial_{12}) + A(l_1, l_2) Y_{l_1 l_2}^{l_1-1, l_2+1} (\partial_2 + \partial_{12}) \\ - (l_1, l_2) Y_{l_1 l_2}^{l_1 l_2} \partial_{12} + Y_{l_1 l_2}^{l_1-1, l_2-1} [B(l_1, l_2) r_1^2 \\ \times (\partial_1 + \partial_{12}) + [B(l_1, l_2) r_2^2 (\partial_2 + \partial_{12}) \\ + C(l_1, l_2)]\} F + Y_{l_1 l_2}^{l_1 l_2} (\nabla_1 \cdot \nabla_2) F. \quad (9b) \end{aligned}$$

For the functions depending on internal degrees of freedom, the Hylleraas coordinates (r_1, r_2, r_{12}) , the ∇ operators may be expressed by

$$\nabla_{r_1} = \frac{r_1}{r_1} \frac{\partial}{\partial r_1} + \frac{r_1 - r_2}{r_{12}} \frac{\partial}{\partial r_{12}},$$

that brings

Thus the kinetic energy operator can be expressed as

$$\nabla_{r_1}^2 F(r_1 r_2 r_{12}) = \left\{ \left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} \right] + \frac{r_1^2 + r_{12}^2 - r_2^2}{r_1 r_{12}} \right.$$

$$\times \frac{\partial^2}{\partial r_1 \partial r_{12}} + \left. \left[\frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}} \frac{\partial}{\partial r_{12}} \right] \right\} F(r_1 r_2 r_{12}), (10.a)$$

$$O_0 = \frac{k_{13}}{2} \left[\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} \right] + k_3 \frac{r_1^2 + r_2^2 - r_{12}^2}{r_1 r_2}$$

$$\times \frac{\partial^2}{\partial r_1 \partial r_2} + \frac{k_{23}}{2} \left[\frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} \frac{\partial}{\partial r_2} \right]$$

$$+ k_2 \frac{r_{12}^2 + r_2^2 - r_1^2}{2 r_2 r_{12}} \frac{\partial^2}{\partial r_{12} \partial r_2} + \frac{k_{12}}{2} \left[\frac{\partial^2}{\partial r_{12}^2} + \right.$$

$$\left. + \frac{2}{r_2} \frac{\partial}{\partial r_{12}} + k_1 \frac{r_1^2 + r_{12}^2 - r_2^2}{2 r_1 r_{12}} \frac{\partial^2}{\partial r_{12}^2} \right]$$

$$O_1 = Y_{LM}^{l_1 l_2} [k_{13} l_1 \partial_1 + k_{23} l_2 \partial_2 + (k_1 l_1 + k_2 l_2) \partial_{12}] F,$$

$$O_2 = A(l_1, l_2) Y_{LM}^{l_1 - l_2 - 1} [k_3 \partial_2 - k_1 \partial_{12}] F,$$

$$O_3 = A(l_1, l_2) Y_{LM}^{l_1 + l_2 - 1} [k_3 \partial_1 - k_2 \partial_{12}] F,$$

$$O_4 = Y_{LM}^{l_1 - l_2 - 1} \{ [k_3 B(l_1, l_2) r_2^2 \partial_2 + C(l_1, l_2) + B(l_1, l_2) r_1^2 \partial_1] - k_1 B(l_1, l_2) r_2^2 \partial_{12} - k_2 B(l_1, l_2) r_1^2 \partial_{12} \} F. \quad (10.b)$$

where $k_i = 1/m_i$, $k_{ij} = k_i + k_j$.

4. Results. In our calculations for the helium ground state five basis sets with independently optimized variational parameters have been used. The construction of the total variational wave function resembles a pine tree. The first layer has been tuned to approximate the general behaviour of the solution at intermediate and large r_1 and r_2 . The second layer is taken to be flexible in a smaller region of r_1 and r_2 , third set is for yet much smaller region, etc. A detailed optimization has been performed for the 5 sets with total $N = 3400$. Quadruple precision is not sufficient at these and larger N and we have used the sextuple precision. Further calculations with

$N = 4600-5200$ have been performed with 64 significant decimal digits (octuple precision) and only partial optimization of variational parameters of the last layer, which approximates a very tiny region around nucleus. Some optimization of a distribution of n_i between the layers $N = (n_1 + n_2 + n_3 + n_4 + n_5)$ has been made as well.

As can be seen from Table 2 presented result extends the accuracy of the nonrelativistic ground state energy for the helium atom substantially.

Second case is the hydrogen molecular ion ground state that represent another limit of mass configuration of constituents with one light and two heavy particles. For this case it is especially essential that complex exponents are introduced, because it is the most natural way to reproduce the oscillatory behaviour of the wave function of the vibrational states. In this case (see Table 3) octuple precision arithmetics has been used to provide the numerical stability of the calculations. Table 4 demonstrates progress in numerical study of the nonrelativistic energy for this state. In Table 5 the other examples are summarized. A negative positronium ion demonstrates a limit of three particles of equal masses. The second and third cases are applications of the method to the states with nonzero angular momentum. The last example in this Table is of special interest. This is the last vibrational state in a series of S -states of the hydrogen molecular ion, and that is the first variational confirmation of the existence of this state (the binding energy corresponding to the cited value is $0,7442251630(4) \text{ cm}^{-1}$. That is probably one of the most spectacular demonstrations of the power of the exponential variational method with complex exponents.

Table 1. Nonrelativistic energies for the ground state of a helium atom ${}^4\text{He}$. N is the number of basis functions. The last digits of the difference in energy between two successive calculations is shown in a third column

N	E_n (in a.u)	ΔE
3400	-2.9037243770341195983110931	
3800	-2.9037243770341195983111421	490
4200	-2.9037243770341195983111540	119
4600	-2.9037243770341195983111572	32
5200	-2.9037243770341195983111587	15
extrap	-2.9037243770341195983111594(4)	

Table 2. Comparison of the ground state energy of the helium atom obtained in this work with other theoretical calculations

	N	E (a.u.)
Frankowski and Pekeris [3]	246	-2.9037243770326
Drake and Yan [4]	262	-2.90372437703411948
Drake [4]	2114	-2.903724377034119596
Korobov [1]	5200	-2.9037243770341195983111594

Table 3. Variational energy (in a.u.) of the positive hydrogen ion ground state as a function of N , the number of basis functions

N	E_n (in a.u.)
3000	-0.5971390631234050747995465
4000	-0.5971390631234050748325657
5000	-0.5971390631234050748340536
6000	-0.5971390631234050748341212
7000	-0.5971390631234050748341327
extrap	-0.597139063123405074834135(3)

Table 4. Comparison of the ground state energy of the positive hydrogen molecular ion obtained in this work with other theoretical calculations.

$$m_p = 1836.152701m_e.$$

	N	E (a.u.)
Gremaud, Delande and Billy [12]	31746	-0.597139063123
Rebane and Filinsky [13]		-0.59713906312340
Moss [14]		-0.5971390631234
This work	7000	-0.5971390631234060748341327

Table 5. Other examples of three-body calculations. (L is the total angular momentum, v is the vibrational quantum number)

System		E
$e^-e^-e^+$	This work [15]	-0.2620050702329801077(3) -0.262005070232976
He (2^3P)	This work [16]	-2.13316419077928310(2) -2.13316419077927
$^4\text{He}^-\bar{p}$ ($L=35$, $v=0$)	This work [17]	-2.98402095449725(1) -2.98402094
$\text{H}_2^+(L=0$, $v=19)$	This work [18]	-0.499731230655812(2) -0.49973123063

5. Conclusions. One may say that this high accuracy is redundant and has no physical meaning. But obviously, it shows the power of modern computers and their ability to solve the quantum three-body problem to any required accuracy. On the other hand, uncertainty in the variational wave function approximately equals the square root of the uncertainty in the variational energy and thus is about 10^{-10} – 10^{-12} . This accuracy does not look redundant. These results prove that the nonrelativistic bound state three-body problem is now satisfactorily solved and the main efforts should be addressed to relativistic and QED effects.

The other advantage of the method is the simplicity of the basis functions that allows for evaluate analytically relativistic matrix elements of the Breit Hamiltonian (see, for example, Ref. [19]). It is possible as well to evaluate analytically the vacuum polarization term (Uehling potential) [20] and to build up an effective numerical scheme for the one-loop self-energy corrections [21]. These features make the considered variational method to be highly powerful universal tool for studying the three-body problem.

A Integrals. Integration over angular variables may be carried out as follows

$$I(r_1, r_2) = \int Y_{LM'}^{l_1 l_2}(r_1, r_2) Y_{LM'}^{l_1' l_2'}(r_1, r_2) d\Omega. \quad (11)$$

Using the expansion from the Appendix B one can get after integration over Euler angles that the only nonzero contribution comes from bipolar harmonics of this expansion with total angular momentum zero,

$$\{Y_l(r_1) \otimes Y_l(r_1)\}_{00} = \frac{(-1)^l (2l+1)^{1/2}}{4\pi} P_l(\cos\theta_{12}).$$

Where $\cos\theta_{12} = (r_1^2 + r_2^2 - r_{12}^2)/(2r_1 r_2)$. It implies that $L' = L''$ and $M' = -M''$. For the variational expansion (4) the angular integral is

$$\begin{aligned} I(r_1, r_2) &= \int [Y_{LM'}^{l_1 l_2}] Y_{LM'}^{l_1' l_2'} d\Omega = \\ &= (-1)^{l_1^2 + l_2^2 - L + M} \int Y_{L-M}^{l_1 l_2} Y_{LM}^{l_1' l_2'} d\Omega. \end{aligned}$$

The coefficient in front of Y_{00}^H in that case is expressed as (see, say, [10])

$$\alpha_i = \frac{(-1)^{l_1' + l_2' - L + M}}{4\pi} (2L + 1) \times \sqrt{(2l_1' + 1)(2l_2' + 1)(2l_1'' + 1)(2l_2'' + 1)} \times C_{L-MLM}^{00} C_{l_1' 0 l_1' 0}^{l_0} C_{l_2' 0 l_2' 0}^{l_0} \begin{Bmatrix} l_1' & l_1' & l \\ l_2' & l_2'' & l \\ L & L & 0 \end{Bmatrix},$$

Using relations

$$\begin{Bmatrix} l_1' & l_1' & l \\ l_2' & l_2'' & l \\ L & L & 0 \end{Bmatrix} = \frac{(-1)^{l_1'' + l_2' + l + L}}{\sqrt{(2L + 1)(2l + 1)}} \begin{Bmatrix} l_1' & l_1'' & l \\ l_2'' & l_2' & L \end{Bmatrix},$$

$$C_{L-MLM}^{00} = \frac{(-1)^{L+M}}{\sqrt{2L + 1}},$$

$$C_{l_1' l_1' 0}^{l_0} = (-1)^{l_1' - l_1''} \sqrt{2l + 1} \begin{Bmatrix} l_1' & l_1'' & l \\ 0 & 0 & 0 \end{Bmatrix},$$

$$C_{l_2' l_2' 0}^{l_0} = (-1)^{l_2' - l_2''} \sqrt{2l + 1} \begin{Bmatrix} l_2' & l_2'' & l \\ 0 & 0 & 0 \end{Bmatrix},$$

one eventually gets:

$$\alpha_i = \frac{(-1)^L}{4\pi} \sqrt{(2l_1' + 1)(2l_2' + 1)} \times \sqrt{(2l_1'' + 1)(2l_2'' + 1)(2l + 1)} \times \begin{Bmatrix} l_1' & l_1'' & l \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_2' & l_2'' & l \\ 0 & 0 & 0 \end{Bmatrix} \begin{Bmatrix} l_1' & l_1'' & l \\ l_2'' & l_2' & L \end{Bmatrix} \quad (12)$$

After averaging over rotational angles the matrix element calculations will be reduced to some linear combinations of integrals of the type

$$\Gamma_{lmn}(\alpha, \beta, \gamma) = \iiint r_1^i r_2^m r_{12}^n e^{-\alpha r_1 - \beta r_2 - \gamma r_{12}} dr_1 dr_2 dr_{12} \quad (13)$$

over internal degrees of freedom, where (i, m, n) is a set of integers, in general, nonnegative integers but for some particular (singular) cases one of indices or even two of them can be negative. In particular, all the terms in the Breit Hamiltonian are of singular

type, while operators of the nonrelativistic Hamiltonian are of regular type.

Integrating by parts it can be easily established that

$$\left(-\frac{\partial}{\partial \alpha}\right) \Gamma_{l-1, mn}(\alpha, \beta, \gamma) = \Gamma_{lmn}(\alpha, \beta, \gamma) \quad (14)$$

and thus, all $\Gamma_{lmn}(\alpha, \beta, \gamma)$ for nonnegative (l, m, n) can be generated from

$$\Gamma_{000}(\alpha, \beta, \gamma) = \frac{2}{(\alpha + \beta)(\beta + \gamma)(\gamma + \alpha)}. \quad (15)$$

A general recurrence scheme has been introduced in [22], which we reproduce here for the convenience of reading in its original form,

$$\Gamma_{lmn} = \frac{1}{\alpha + \beta} [l \Gamma_{l-1, mn} + m \Gamma_{l, m-1, n} + B_{lmn}]$$

$$B_{lmn} = \left(-\frac{\partial}{\partial \alpha}\right)^l \left(-\frac{\partial}{\partial \beta}\right)^m \left(-\frac{\partial}{\partial \gamma}\right)^n \frac{2}{(\alpha + \gamma)(\beta + \gamma)};$$

$$B_{lmn} = \frac{1}{\alpha + \gamma} [l B_{l-1, mn} + n B_{l, m-1, n} + A_{lmn}]$$

$$A_{lmn} = \left(-\frac{\partial}{\partial \alpha}\right)^l \left(-\frac{\partial}{\partial \beta}\right)^m \left(-\frac{\partial}{\partial \gamma}\right)^n \frac{2}{(\beta + \gamma)}$$

$$= \delta_{l0} \frac{2(m+n)}{(\beta + \gamma)^{m+n+1}}. \quad (16)$$

This recursion is numerically stable since all the quantities which appear in the recurrence formulas are nonnegative.

B. Bipolar harmonics. For a product of two bipolar harmonics one has

$$\{Y_{l_1}(r_1) \otimes Y_{l_2}(r_2)\}_{LM'} \{Y_{l_1}(r_1) \otimes Y_{l_2}(r_2)\}_{LM''} = (17)$$

$$= \sum_{LM} C_{LM}^{LM} \sum_{l_1 l_2} B_{l_1 l_2 L}^{l_1 l_2 L} \{Y_{l_1}(r_1) \otimes Y_{l_2}(r_2)\}_{LM},$$

where

$$B_{l_1 l_2 L}^{l_1 l_2 L} = \sqrt{\frac{(2l_1' + 1)(2l_2' + 1)(2l_1'' + 1)}{(4\pi)^2}} \times \sqrt{(2l_2'' + 1)(2L' + 1)(2L'' + 1)} \times C_{l_1' 0 l_1' 0}^{l_0} C_{l_2' 0 l_2' 0}^{l_0} \begin{Bmatrix} l_1' & l_1' & l_1 \\ l_2' & l_2'' & l_2 \\ L' & L'' & L \end{Bmatrix} \quad (18)$$

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Резюме

Кулондық үшденелі байланысқан күйді зерттеуге арналған ең күшті әдіс ретінде вариациялық әдісті қолданамыз. Бұл жұмыста вариациялық базисті комплекті көрсеткіштермен экспоненциалды корреляциялады. Осы жұмыста көрсеткендей, бұл әдіс көптеген белгілі атомдық және молекулалық жүйелерге арналған байланысты күйдегі энергияларды береді.

Резюме

Известно, что вариационные методы являются наиболее мощным инструментом для изучения кулоновского трехтельного связанного состояния. В данной работе экспоненциально явно коррелировали вариационный базис типа с комплексными показателями. Как было показано, что этот метод дает энергии связанных состояний для многих известных атомных и молекулярных систем.

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