Heron Variables in 3-body Coulomb Problem

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Abstract
The use of coordinate variables with independent physical boundaries – Heron variables – is proposed for the 3-body problem. The ansatz is given for variational trial wave functions without local energy infinities at the Coulomb singularities.

Introduction. Heron variables
The wave function of a bound system in a ground state depends only on interparticle distances. There are three distances \( r_1, r_2 \) and \( r_3 \) for 3-body systems, six for 4-body and so on. Though the distances are locally independent and admit unconstrained partial differentiation, the physical boundaries for each of them depend on the values of the others. The triangle inequalities take place:

\[
0 \leq |r_2 - r_3| \leq r_1 \leq r_2 + r_3 < \infty,
\]

\[
0 \leq |r_1 - r_3| \leq r_2 \leq r_1 + r_3 < \infty,
\]

\[
0 \leq |r_1 - r_2| \leq r_3 \leq r_1 + r_2 < \infty.
\]

(1)

More symmetrical Hylleraas variables

\[
s = r_1 + r_2, \quad t = |r_1 - r_2|, \quad u = r_3
\]

(2)

are used for decades in the variational calculations of the 3-body systems. These variables are also subjected to the physical region inequalities:

\[
0 \leq t \leq u \leq s < \infty.
\]

(3)

All such variables with mutual constraints are not fully independent, and this causes definite technical difficulties in calculations.

Meanwhile, there are coordinate variables with independent physical boundaries. They are known for millenniums since the discovery by Heron (Alexandria, 1st century A.D.) of the triangle area formula

\[
S = \sqrt{p(p-a)(p-b)(p-c)}, \quad p = (a + b + c)/2.
\]

(4)

The Heron variables

\[
p - a = h_1 = (-r_1 + r_2 + r_3)/2,
\]

\[
p - b = h_2 = (r_1 - r_2 + r_3)/2,
\]

\[
p - c = h_3 = (r_1 + r_2 - r_3)/2
\]

(5)

span separately over the physical region

\[
0 \leq h_1 < \infty, \quad 0 \leq h_2 < \infty, \quad 0 \leq h_3 < \infty.
\]

(6)

They are fully independent, that leads to great simplification in variational calculations. The repeated integrals turn to multiple integrals, which reduce to one-dimensional integrals, if the trial wave functions are appropriately chosen.

The equivalent variables, without referring to Heron and now usually named as perimetric variables, were proposed in [3] and effectively used in [4] and other works.

[1] The updated version of the talk published in the Proceedings of the XI International Workshop on High Energy Physics and Quantum Field Theory, 12-18 September 1996, St.-Petersburg, Russia, pp. 403-405. Ed. by B.B.Levtchenko, Moscow, 1997.
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[3] The author is indebted to G. W. F. Drake for these references.
1 Ansatz for variational trial wave functions

For Helium and Helium-like ions the simplest ground state function can be chosen as follows:

\[ \psi = \exp(-Zr_1 - Zr_2 + r_3/2). \]  

(7)

If an electron pair were isolated, the exact solution \( \psi_{ee} = \exp(r_3/2) \) of the Schrödinger equation with repulsive Coulomb potential would be unphysical because of unrestricted exponential growth. Being embedded into the wave function of a whole bound system, the exponent with the plus sign in front of \( r_3 \) does not produce unrestricted exponential growth in the 3-body configuration space. Transition to Heron variables

\[ r_1 = h_2 + h_3, \quad r_2 = h_1 + h_3, \quad r_3 = h_1 + h_2 \]  

(8)

exposes exponential decrease on each variable:

\[ \psi = \exp(-(Z - 1/2)h_1 - (Z - 1/2)h_2 - 2Zh_3). \]  

(9)

The mean energy value, calculated with this function is

\[ H_{\text{mean}} = -\frac{(1 + 2Z)(1 - 8Z + 28Z^2 - 64Z^3)}{4(-1 + 10Z - 32Z^2)}. \]  

(10)

This value is obtained without any parameters for adjustment, as at this lowest level of approximation no minimization procedure was performed.

It is instructive to compare the approximation qualities of the proposed wave function with that of the variational wave function with one adjustable parameter – the effective charge:

\[ Z_{\text{eff}} = Z - 5/16, \quad \psi_{\text{eff}} = \exp(-Z_{\text{eff}}r_1 - Z_{\text{eff}}r_2). \]  

(11)

The one parameter mean energy value

\[ H_{\text{mean}}(Z_{\text{eff}}) = -(Z - 5/16)^2 \]  

(12)

shows for all \( Z \) only a little bit bigger deviation from the energy eigenvalues, as the parameterless formula (7) does, but the local properties of \( \psi_{\text{eff}} \) are much worse than that of \( \psi \).

The so-called local energy, defined as

\[ E_{\text{local}} = H\psi_{\text{eff}}/\psi_{\text{eff}}, \]  

(13)

takes infinite values at the Coulomb singularities [1].

On the contrary, the local energy, attributed to the proposed function [7], has bounded variation in the whole physical region of variables.

As one can judge with the known literature, almost all used up to now variational wave functions are plagued with the local energy infinities, in spite of the huge number of their parameters.

How to avoid local energy infinities at any approximation stage? The simplest ansatz for good trial function is suggested on by the presented example of the wave function in the lowest approximation. It is sufficient to have a linear superposition of triple products, formed by the exact Coulomb solutions for each pair of the particles involved.

The building blocks are:

\[ \psi(n, l = 0) = \exp(-ar/n) \frac{1}{_1F_1(1-n, 2, 2ar/n)}, \]

\[ \psi(n, l = 1) = r_1 \exp(-ar/n) \frac{1}{_1F_1(2-n, 4, 2ar/n)}, \]

\[ \psi_{ij}(n, l = 2) = (\delta_{ij}r_i^2 - 3r_1r_2) \exp(-ar/n) \frac{1}{_1F_1(3-n, 6, 2ar/n)}, \]  

(14)

In (14) \( r = r_1, r_2, \) or \( r_3, \) \( n = n_1, n_2, \) or \( n_3 \) and \( a = Z, \) or \( a = -1/2 \) correspondingly.

The individual principal quantum number \( n \) need not to be integer, and can be treated as an adjustable parameter in a truncated hypergeometrical series. Each term of the linear superposition should not violate the condition of integral convergence: \( \text{Max}(n_1, n_2) < 2Zn_3. \) The intermediate vector indices should be summed in all possible ways according to transformation properties of the whole system state. And the symmetrization or antisymmetrization on the variables \( r_1, r_2 \) should be performed.
2 Axial states of a 3-body system

Let’s apply the proposed ansatz to the 3-body state, when the relative angular momenta of each pair of particles form an overall $P$-state with positive parity – the axial state.

In the lowest approximation the axial wave function is

$$\tilde{\psi}_i = \exp(-Zr_1/2 - Zr_2/2 + r_3/4)\epsilon_{ijk}r_{1j}r_{2k}. \tag{15}\label{eq:psi}$$

The mean energy value is calculated as

$$H_{\text{ax mean}} = \frac{(-1 + 2Z)(-1 + 14Z - 84Z^2 + 280Z^3 - 512Z^4)}{16(-1 + 16Z - 100Z^2 + 256Z^3)}. \tag{16}\label{eq:Haxmean}$$

Though the energy level of this doubly excited state is well above the ground level, the axial state is stable against autoionization. For symmetry reasons, the autoionization of an axial state cannot proceed to the final 2-body ground state, which is scalar state. For energy reasons, it also cannot proceed to the final 2-body $2P$-state, that follows from the lowest approximation formula (16) for $Z > 1$ and was established for the Hydrogen negative ion in [6].

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