Three-body bound-state problem with Coulomb forces*

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(Received 26 January 1976)

The three-body bound-state problem with Coulomb forces is solved in the Feshbach-Rubinow approximation. Analytical expressions for the ground-state energy and wave function are obtained, and numerical results are presented for heliumlike atoms.

The nonrelativistic bound-state problem of three charged particles interacting via the bare Coulomb potential has a long history and still continues to be of current interest. There have been two types of approaches: the variational method and the hyperspherical or K-harmonics method. The accuracy of the former method depends on the choice of the trial wave function, and usually one has to deal with a very large number of variational parameters.[1] In the latter method the Schrödinger equation for the three-body system is reduced to an infinite set of coupled differential equations of one variable.

There has been a surge of interest in the K-harmonics approach in recent years.[2-7] It has been found, however, that the convergence of the K-harmonics expansion is quite slow, and a very large number of coupled equations have to be solved numerically to achieve good accuracy.[3] The method that we adopt in this note is a combination of the variational and the differential-equation approach. We assume at the outset that the three-body wave function depends only on a single appropriately chosen variable *containing a few variational parameters*. The three-body bound state problem then reduces to the solving of a *single* second-order differential equation. Moreover, the solution of this equation can be found *analytically*. As an illustration, we apply the method to the two-electron atomic systems like H^-, He, Li^+, etc., and obtain the wave function analytically. Our numerical result for the ground-state energy of He atom is comparable in accuracy to the more elaborate computer calculations of Ref. 3.

The method that we outline here was originally proposed in its simplest form in the three-body nuclear problem by Feshbach and Rubinow,[8] and was later generalized by other authors.[9,10] Here we apply the formalism to the pair-wise Coulomb interaction, where the resulting formulas become particularly simple. Consider three particles of masses m_i and charges $Z_i e$ ($i = 1, 2, 3$) interacting through Coulomb potentials alone. Assume that the wave function of the three-body system is a function of the single non-negative variable R,

$$\Psi = \Phi(R), \quad R = \tfrac{1}{2}(\eta_1 r_1 + \eta_2 r_2 + \eta_3 r_3) \ . \tag{1}$$

Here r_1 is the interparticle distance between particles 2 and 3, and likewise for r_2 and r_3, while η_1, η_2, and η_3 are variational parameters, with the restrictions[11] that $\eta_1 + \eta_2 > 0$, $\eta_2 + \eta_3 > 0$, and $\eta_3 + \eta_1 > 0$. The expectation value of the three-body Hamiltonian H, $\langle\Phi|H|\Phi\rangle$, may then be reduced to a single integral over the variable R, and application of the condition $\delta\{\langle\Phi|H|\Phi\rangle/\langle\Phi|\Phi\rangle\} = 0$ yields the Schrödinger-like equation[8,10]

$$-\frac{\hbar^2}{m}\frac{d^2u}{dR^2} + \mathcal{U}(R)\,u = 8\xi E u \ , \tag{2}$$

where E is the energy, and

$$u(R) = R^{5/2}\Phi(R) \ , \tag{3}$$

$$m^{-1} = \xi \sum_{\text{cycl}} (\eta_1^2 + \eta_2^2) m_3^{-1} + \zeta \eta_1 \eta_2 \eta_3 \sum_i (m_i^{-1}) \ , \tag{4}$$

$$\mathcal{U}(R) = \frac{\hbar^2}{m}\frac{15}{4R^2} + 4\sum_i W_i(R) \ . \tag{5}$$

Explicit forms for ξ, ζ, and $W_i(R)$ are as follows:

$$\xi = \frac{2^5[(\eta_1+\eta_2+\eta_3)^3 + \eta_1\eta_2\eta_3]}{15[(\eta_1+\eta_2)(\eta_2+\eta_3)(\eta_3+\eta_1)]^3} \ , \tag{6}$$

$$\zeta = \frac{2^6[(\eta_1+\eta_2+\eta_3)^2 + \eta_1\eta_2 + \eta_2\eta_3 + \eta_3\eta_1]}{15[(\eta_1+\eta_2)(\eta_2+\eta_3)(\eta_3+\eta_1)]^3} \ , \tag{7}$$

$$W_1(R) = \frac{Z_2 Z_3 e^2}{R}\frac{16}{3} \times \frac{(\eta_2+\eta_3)(2\eta_1+\eta_2+\eta_3) + \eta_1^2 + \eta_2\eta_3}{(\eta_1+\eta_2)^2(\eta_2+\eta_3)^3(\eta_3+\eta_1)^2} \ . \tag{8}$$

The expressions for W_2 and W_3 are obtained by cyclic permutations of the indices in Eq. (8). Although the equations are formidable looking, the main point to note is that $\sum_i W_i(R)$ still varies as R^{-1}; so Eq. (2) is simply a one-body Schrödinger equation with a Coulomb potential and a centrifugal potential term corresponding to the orbital quantum number $l = \frac{3}{2}$. The expressions for eigenenergies and eigenfunctions in terms of the varia-

tional parameters η_i may therefore be analytically expressed.

As an example, consider a two-electron atomic system with a nuclear charge Ze, and for simplicity assume the nuclear mass to be infinite. Designating the two electrons as particles 1 and 2, define the variable R by the equation

$$R=\tfrac{1}{2}(r_1+r_2+\eta r_3),$$

with the restriction that $1+\eta>0$. For this situation, using Eq. (8), we obtain

$$4\sum_i W_i(R)=-\frac{e^2}{R}\,\frac{8[(16Z-5)+4\eta(Z-1)-\eta^2]}{3(1+\eta)^4}\,. \tag{9}$$

A little algebra yields the differential equation for u:

$$\frac{\hbar^2}{2m_0}\left(-\frac{d^2}{dR^2}+\frac{15}{4R^2}\right)u-\frac{e^2}{R}\,\frac{5[(16Z-5)+4\eta(Z-1)-\eta^2]}{2(8+7\eta+4\eta^2+\eta^3)}\,u=\frac{2(8+5\eta+\eta^2)}{(1+\eta)(8+7\eta+4\eta^2+\eta^3)}\,Eu\,, \tag{10}$$

where m_0 is the electron mass. Since this is just the wave equation with a Coulomb potential for an effective orbital momentum state $l=\frac{3}{2}$, we can immediately write down the energy and eigenfunction for the ground state (with the principal quantum number $n=\frac{5}{2}$). In atomic units of $m_0e^4/\hbar^2$, the ground-state energy is

$$E_0=-\frac{(1+\eta)[(16Z-5)+4\eta(Z-1)-\eta^2]^2}{4(8+5\eta+\eta^2)(8+7\eta+4\eta^2+\eta^3)}\,, \tag{11}$$

and the ground-state wave function is

$$\Phi_0(R)=R^{-5/2}u_0(R)$$

$$=\exp\left(-\frac{(16Z-5)+4\eta(Z-1)-\eta^2}{8+7\eta+4\eta^2+\eta^3}\,\frac{R}{a}\right), \tag{12}$$

where $a=\hbar^2/m_0e^2$ is the Bohr radius. For a given Z, η should be varied in the range $-1<\eta<\infty$ to find the minimum in E_0 from Eq. (11). Using this procedure for H^-, He, Li^+, and Be^{++}, we find $-E_0$ in atomic units to be 0.508 (0.528), 2.890 (2.904), 7.267 (7.280), and 13.643 (13.656), respectively, where the numbers in parentheses are the best nonrelativistic estimates,[12] which we have rounded off to three decimal figures for comparison. The optimum values of η's which minimize the ground-state energies for $Z=1$ to 4 are -0.264, -0.138, -0.092, and -0.070, respectively. Our results are consistently better than the simplest conventional one-parameter variational calculation, where H^- is not found to be bound. The latter method[13] gives $E_0=-(Z-\frac{5}{16})^2$, which is what we would obtain from Eq. (11) on setting $\eta=0$. Our method, which is also variational, yields better results because the interelectronic distance r_3 is taken explicitly into account in the wave function. Taking this variable in the exponent, as we do, may be an efficient way to parametrize the wave function, as the work of Radi[1] shows.

Finally, in comparing our method to the hyperspherical or K-harmonics calculations, note that if only the $K=0$ component of the wave function is retained, the problem also reduces to solving a single differential equation in the variable $\rho\equiv(r_1^2+r_2^2+r_3^2)^{1/2}$, instead of our R. This equation, in the nuclear problem of the model triton, was first solved by Morpurgo.[14] McMillan,[15] comparing the Morpurgo and the Feshbach-Rubinow equations, showed that the latter yielded significantly better numerical results in the triton. The Morpurgo equation, however, has the advantage that it can be systematically improved through the K-harmonics formalism. Since in our method already the zeroth-order results are reasonably good, it would be worthwhile if a similar systematic way of improving it could be found.

The authors acknowledge many useful discussions with Dr. Jimmy Law.

*Research supported by the National Research Council of Canada.

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