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System-adapted contours and the Feshbach-Rubinow method

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A generalization of the Feshbach-Rubinow method for variationally determining the ground-state energy of a multiparticle system is described and applied to the H^- ion. The method finds a variationally optimized function of a contour that characterizes the system. The contour can be quite complicated, being itself determined by some approximation scheme for solving the multiparticle Schrödinger equation. The application to the H^- ion uses an already optimized three-parameter contour due to Bethe, and a significant improvement in the ground-state energy is noted.

I. INTRODUCTION

The Feshbach-Rubinow (FR) single-variable variational method[1] has been applied to the three-body problem by a number of authors.[2] The method involves finding an optimum function of a variable u constructed from the interparticle distance. These authors use the contour

$$u=(\eta_1 r_1+\eta_2 r_2+\eta_3 r_3)\ ,$$

where, for example, r_1 is the distance between particles 2 and 3, and η_1, η_2, and η_3 are variational parameters.

We extended this techique by constructing an optimized symmetrized function of the variable u,[3] and the calculation showed that symmetrization improves the estimation of the ground-state energy of the H^- ion.

It is not obvious, however why the above choice for u is a sensible starting point. The solution of the multidimensional Schrödinger equation for the many-particle system may be approached either variationally or perturbatively. Either technique establishes a set of contours $u(\vec{r}_1,\vec{r}_2,\vec{r}_3,\ldots,)$ which might be a better choice than the FR contour.

We propose to present a technique which variationally establishes the optimum function of the contours u. The new function satisfies an ordinary differential equation that is readily solved numerically. This is a generalization of the FR method because the contours u can have almost any degree of complexity.

II. THREE-BODY SYSTEMS

The Schrödinger equation for the S state of the three-body system is

$$\sum\left\{-\frac{\hbar^2}{2}\left[\left(\frac{1}{m_2}+\frac{1}{m_3}\right)\left(\frac{\partial^2}{2r_1^2}+\frac{2}{r_1}\frac{\partial}{\partial r_1}\right)+\frac{1}{m_1}\frac{r_2^2+r_3^2-r_1^2}{r_2r_3}\frac{\partial^2}{\partial r_2\partial r_3}\right]+V_1(r_1)\right\}\times\psi(r_1,r_2,r_3)=E\psi(r_1,r_2,r_3)\ , \tag{1}$$

with central interparticle potentials $V_i(r_i)$ and particle masses m_i. The sum is over the cyclic permutations of the interparticle distances r_i.

In the FR approach, the wave function is approximated by a variationally determined function of the simple contour given in the introduction. Various applications of this method have been made, as in Refs. 2, with reasonably good results. Slight changes in the contour, see Srivastava *et al.*,[4] lead to improved results. Greater flexibility is achieved by Lie, Nogami, and Preston[5] by taking

$$\psi(r_1,r_2,r_3)=\phi(r_3)\exp[-(\alpha r_> +\beta r_<)] ,$$

and variationally obtaining the function $\phi(r_3)$.

Our plan is to retain the spirit of the FR approach but allow the contour to take a form better adaped to the system. For heliumlike systems, in which inverse-square forces bind the components, a reasonable contour might be

$$u=\exp(-c_1r_1-c_2r_2-c_3r_3)\left[\sum_{ijk}c_{ijk}r_1^i r_2^i r_3^k\right] , \tag{2}$$

which could be appropriately symmetrized for idential particles. This contour could be optimized by an initial application of the variational principle to determine the constants c. After this optimization of u, a second application of the variational principle is used to determine the best function $f(u)$. This is accomplished by requiring that

$$E=\frac{\int fHf\,d\tau}{\int f^2 d\tau} \tag{3}$$

be stationary with respect to variations of f. Here, H is the Hamiltonian given in Eq. (1). Thus, the function $f(u)$ must satisfy

$$\int(\delta fHf)d\tau+\int(fH\delta f)d\tau=2\tilde{E}\int\delta ff\,d\tau . \tag{4}$$

The next section presents an example to illustrate the technique.

III. THREE-BODY SYSTEM WITH TWO IDENTICAL COMPONENTS

In an early study, Bethe[6] suggested that the ground state of the two electron heliumlike ions can be approximated with three-parameter functions of the form

$$u(r_1,r_2,r_3)=e^{-ks/2}(1+c_1ks\omega+c_2k^2s^2t^2\omega^2) , \tag{5}$$

where

$$s=r_1+r_2,\quad w=r_3/(r_1+r_2) ,$$

$$t=(r_1-r_2)/r_3 ,$$

and r_1 r_2, and r_3 are the interparticle distances. Application of the variational principle yields $k=1.535$, $c_1=0.20$, and $c_2=0.05$. the resulting variational energy for the bound state is $E=-0.5253$ a.u.

We now wish to establish the best function of u, $f(u)$ by solving Eq. (4). To do so, the space of integration must be spanned by three variables one of which is u; i.e., $(s,w,t)\rightarrow(u,s,t)$, (u,w,t), or (u,s,w). We illustrate the technique by taking the Bethe form of Eq. (5). As

$$0\le w\le 1,\quad 0\le t\le 1,\quad c_1\le 0.5$$

and

$$c_2<0.125 ,$$

$$1+c_1kws+c_2k^2w^2s^2t^2\le e^{ks/2} ,$$

which implies $0\le u\le 1$. This observation allows to transform the integrals of Eq. (4) to integrals in (u,w,t) space. The results for the various terms of Eq. (4) are

$$\int_0^\infty\int_0^1\int_0^1 f^2 d\tau=\int_0^1\int_0^1\int_0^1 f^2(u)\left|\frac{\partial s}{\partial u}\right|s^5w^2(1-w^2t^2)du\,dw\,dt ,$$

$$\int_0^\infty\int_0^1\int_0^1 fHf\,d\tau=\int_0^1\int_0^1\int_0^1\left[\frac{1}{2}\left[\frac{df}{du}\right]^2(\vec{\nabla}_1u\cdot\vec{\nabla}_1u+\vec{\nabla}_2u\cdot\vec{\nabla}_2u)+f^2V\right]$$

$$\times\left|\frac{\partial s}{\partial u}\right|[s^5w^2(1-w^2t^2)du\,dw\,dt] . \tag{7}$$

The potential V staisfies the equation

$$\begin{aligned}V(u,w,t)&=-1/r_1-1/r_2+1/r_3\\&=\frac{-r_3(r_1+r_2)+\vec{r}_1\cdot\vec{r}_2}{r_1r_2r_3}\\&=\frac{-4s^4w^2+s^4w(1-w^2t^2)}{s^5w^2(1-w^2t^2)} ,\end{aligned} \tag{8}$$

and

$$\begin{aligned}s&=s(u,w,t)\\&=\frac{2}{k}[-\ln u+\ln(1+c_1ksw+c_2k^2w^2s^2t^2)] .\end{aligned} \tag{9}$$

The gradient terms are handled by expressing u in terms of r_1, r_2, and r_3, carrying out the differentiations with respect to the electron coordinates, expressing the results in terms of s,t,w, and finally substituting $s=s(u,w,t)$.

Since s is a transcendential function of the variables u, w, and t exact integrations of Eq. (4) and (7) are not possible. They are evaluated numerically by using a set of 10-G points[7] for the variables w and t; let them be denoted $\bar{w}$ and $\bar{t}$. The variable $s(u,\bar{w},\bar{t})$ is then evaluated by simple iteration of Eq. (7). [For u near unity more iterations are needed; u near zero s goes like $-2/k\ln(u)$.] The derivative term $|\partial s/\partial u|$ is readily evaluated by using Eq. (9).

Thus the integrals (6) and (7) can be performed for the variables t and w, leaving only u. The next step is an application of the variational principle [Eq. (3)]. This leads to the ordinary differential equation

$$\frac{d}{du}\left[p(u)\frac{df}{du}\right]+q(u)f=\tilde{E}r(u)f\ , \tag{10}$$

where

$$\begin{aligned}
p(u)&=-\tfrac{1}{2}\int_0^1\int_0^1\left|\frac{\partial s}{\partial u}\right|(\vec{\nabla}_1u\cdot\vec{\nabla}_1u+\vec{\nabla}_2u\cdot\vec{\nabla}_2u)s^5w^2(1-w^2t^2)dw\,dt\ ,\\
q(u)&=\int_0^1\int_0^1\left|\frac{\partial s}{\partial u}\right|s^4[-4w^2+w(1-w^2t^2)dw\,dt]\ ,\\
r(u)&=\int_0^1\int_0^1\left|\frac{\partial s}{\partial u}\right|s^5w^2(1-w^2t^2)dw\,dt\ .
\end{aligned}\tag{11}$$

Numerical evaluation of p, q, and r reduce the problem to the solution of a relatively straightforward ordinary differential equation.

IV. THE SOLUTION OF EQ. (10)

The variable s given by Eq. (9) has the form

$$s\sim\frac{2(1-u)}{k(1-2c_1w)}\ ,$$

for $u\sim 1$. Thus for u near unity

$$p(u)\sim p_0(u-1)^5,\ \ q(u)\sim q_0(u-1)^4\ ,$$

and

$$r(u)\sim r_0(u-1)^5\ ,$$

so that Eq. (10) tends to the form

$$5p_0f'(1)+q_0f(1)=0\ ,$$

for u near unity. Then using the normalization $f(1)=1$, $f'(1)$ is known, and the differential equation can be solved by dividing the interval $0\le u\le 1$ into ten equally spaced points and solving $f(u)$ at these points, and working inward from $u=1$ by some numerical scheme such as the Runge-Kutta. As the coefficients p, q, and r of Eq. (11) are singular near $u=0$, the process outlined above is carried out to obtain $f(0.1)$. The interval $0\le u\le 0.1$ is again partitioned, and $f(0.01)$ is obtained in the same way. The procedure is continued until $f(0.001)$ is obtained. The value of $\tilde{E}$ is fixed during this procedure. For values of $\tilde{E}$ below the best upper bound, $f(u)$ decreases from $u=1$ then increases for smaller values of u. For values of $\tilde{E}$ above the best upper bound: $f(u)$ decreases from $u=1$, then goes through to zero, and continues to decrease. The best estimate of $\tilde{E}$ produces $f(u)=0$ for u at its minimum value, and the best estimate of $\tilde{E}$ obtained by our present work is -0.5264 a.u.

V. DISCUSSION OF THE NUMERICAL RESULTS

Table I summarizes the results of our analysis. The work of Ref. 3 used a one-parameter contour u to obtain an optimized function $f(u)$ and an energy of -0.522 a.u. for the ground-state energy of H^-. The Bethe variational calculation uses the three-parameter contour given in Eq. (1) with the result -0.5253 a.u. Our method finds the best function of the Bethe u, and the value of E is only slightly improved to -0.5254 a.u. A further search found by varying the Bethe parameters k,

TABLE I. Values of the variationally optimized values for the binding energy of the H^- ion.

Model	$\tilde{E}$ (a.u.)
Best available results, Ref. 8	−0.5277
Results of Ref. 5	−0.5261
Symmetrized two-parameter fit of Ref. 3	−0.5220
Bethe result using a symmetrized three-parameter contour, Ref. 4	−0.5253
Present work using the best function of the Bethe contour	−0.5264

c_1, and c_2 yields the value $E=-0.5264$ a.u. with $k=0.965\,89$, $c_1=0.168\,79$, and $c_2=0.53\,512$. Also given in Table I is the recent result of −0.5261 a.u. obtained by Lie and Nogami (Ref. 5).

The best value of the binding energy of the H^- ion is given by Pekeris.[8] The absolute differences between the Bethe value and our best value compared to the Pekeris result are, respectively, 2.4×10^{-3} and 1.3×10^{-3} a.u. Both methods use the same basic contour containing three variational parameters, but the value of these parameters are quite different. In fact, if our parameters are used in the Bethe contour, the resulting binding energy deteriorates to −0.4458 a.u. The function $f(u)$ corresponding to our best fit is compared to u in Fig. 1.

An observable of some importance is the electron overlap factor $\langle\delta(\vec{r}_3)\rangle$. It is easily evaluated in terms of $f(u)$ as

$$\langle\delta(\vec{r}_3)\rangle\langle f^2\rangle=\frac{4\pi^2}{k^3}\int_0^1 du(\ln u)^2 f^2(u)/u \ . \quad (12)$$

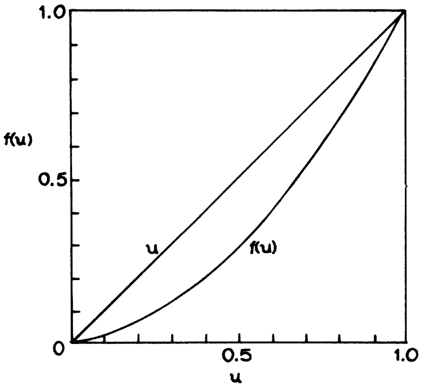

FIG. 1. Plot of the variationally optimized function of the Bethe contour $f(u)$ versus u.

The best value of $\langle\delta(\vec{r}_3)\rangle$ is 2.74×10^{-3} a.u. as calculated in Ref. 8. The value obtained in our best energy fit is 3.52×10^{-3} a.u., while the result from the Bethe contour with out parameters is 9.13×10^{-4} a.u. Lie and Nogami, in Ref. 5, obtained 2.95×10^{-3} and 2.65×10^{-3} a.u., the latter value from their best energy fit.

The size of the electron overlap factor is so small that is remarkable that all these various variational calculations are in reasonable agreement. It is evident that $\langle\delta(\vec{r}_3)\rangle$ is much more sensitive to the variational function than the nicely bounded energy. If one had prior knowledge of $\langle\delta(\vec{r}_3)\rangle$, an especially finely tuned variational function could be obtained.

VI. CONCLUSIONS

This work extends the technique of Feshbach and Rubinow (Ref. 1) and Bhadhuri and Nogami (Ref. 2), by allowing more complex forms for the contours. We applied our technique to the bound state of the H^- ion and obtained a ground-state energy that is in good agreement with the best available result (Ref. 8).

The value of the present work lies in our ability to use contours with complicated forms. The Feshbach-Rubinow approach requires a simple contour that leads to a relatively simple differential equation for the best function of the contour. Such a simple contour may not be evident or adequate. In fact, we could use the much more realistic contour of Lie and Nogami as a starting point for our approach with the guarantee that the second application of the variational principle will lead to an improved wave function.

The technique could be applied to other systems. For example, the helium trimer system can be described by a variety of potential functions that contain a repulsive core. An approximate solution can be constructed by a number of strategies including variational calculations and solution of the Faddeev equations.[9] We could, in principle, use one of these solutions as the system-adapted contour and then find the best function of this contour by the procedures outlined in this paper.

Another application of the technique is in the study of mesonic atoms. For example, muonic helium (a ^{4}He nucleus bound to an electron and a muon) has recently been studied by a number of authors.[10] The hyperfine splitting

$$\Delta\nu=k\int d\vec{x}\,d\vec{r}\,\delta(\vec{x}-\vec{r})\psi^2 \ ,$$

with $\vec{x}$ the muon coordinate and $\vec{r}$ the electron coordinate, requires the knowledge of the ground-state wave function. Huang and Hughes[11] have calculated a highly accurate but complicated solution and Drachman (see Ref. 10) has obtained an analytic first-order wave function. This analytic form defines a set of contours upon which we may establish an optimized function in the manner described above.

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$$\psi=\phi(r_3)[\exp(-\alpha r_1-\beta r_2)+\exp(-\alpha r_2-\beta r_1)] ,$$

with α and β the variational parameters. Their binding energy for the H^- ion is given in Table I: S. G. Lie and Y. Nogami, Can. J. Phys. 58, 760 (1980).

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