A NOTE ON A SOLUBLE THREE-BODY PROBLEM*

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Summary

A class of soluble three-body systems suggested by Pluvinage is studied. The Hamiltonian H_0 of these systems is not Hermitian, and the energy spectrum contains a continuum of bound states. The use of H_0 as a reference Hamiltonian in calculations of the helium atom ground state, as suggested by Pluvinage and Walsh, is discussed in the light of these results.

I. Introduction

The wave function ψ describing an S-state of three interacting spinless particles in the centre-of-mass frame is a function only of three coordinates which define the shape of the triangle formed by the particles. Labelling the position vector of the particles from some arbitrary origin as $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$ we can define the relative coordinates x_{ij}:

$$\mathbf{x}_{ij} = \mathbf{x}_j - \mathbf{x}_i. \tag{1}$$

Then the scalars x_{12}, x_{23}, x_{31}, the three sides of this triangle, are a suitable set of coordinates to describe ψ. We use the notation

$$x_{ij} = r_k, \tag{1a}$$

where, here and throughout this paper,

$$(i,j,k) \text{ is a cyclic permutation of } (1,2,3). \tag{1b}$$

In terms of r_1, r_2, r_3, the wave function ψ satisfies the reduced wave equation

$$(H-E)\psi(r_1, r_2, r_3) = 0, \tag{2a}$$

where

$$H = \sum_{i=1}^{3} \{T_0(r_i) + T_{\mathrm{cross}}(i)\} + V(r_1, r_2, r_3), \tag{2b}$$

where

$$T_0(r_i) = -\frac{\hbar^2}{2\mu_i}\left(\frac{\partial^2}{\partial r_i^2} + \frac{2}{r_i}\frac{\partial}{\partial r_i}\right), \tag{2c}$$

$$T_{\mathrm{cross}}(i) = \frac{\hbar^2}{m_i}\frac{\mathbf{r}_j \cdot \mathbf{r}_k}{r_j r_k}\frac{\partial^2}{\partial r_j \partial r_k}, \tag{2d}$$

and the reduced mass μ_i is given by

$$\mu_i = m_j m_k/(m_j + m_k). \tag{2e}$$

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Separable solutions of (2) would exist for a two-body interaction $v = v(r_1)+v(r_2)+v(r_3)$, were it not for the cross terms T_{cross} in the kinetic energy. We can force the existence of separable solutions by choosing the interaction to be

$$v = u(1)+u(2)+u(3),$$

where

$$u(i) = v_i(r_i)-T_{\text{cross}}(i). \tag{3}$$

With this choice of interaction, equation (2) reads

$$(H_0-E_0)\psi_0(r_1, r_2, r_3) = 0, \tag{3a}$$

where

$$H_0 = \sum_{i=1}^{3} \{T_0(r_i)+v_i(r_i)\}, \tag{3b}$$

which clearly has separable solutions and is hence trivially soluble.

The interaction (3) is *not* a sum of two-body interactions, since $T_{\text{cross}}(i)$ is not a function of r_i only. However, it is possible that, at least for some systems, T_{cross} may be in some sense "small"; and hence (3a) is an attractive starting point for a discussion of the exact equation (2) with a two-body interaction of the form

$$V = \sum_{i=1}^{3} v_i(r_i). \tag{4}$$

Examples of such discussions have already appeared in the literature. Delves and Derrick (1963) have derived a set of equations for choosing a suitable *variational* wave function for (2) in the nuclear problem, which for spinless particles reduce to equation (3a). A similar discussion has been given by Pluvinage (1950), and by Spruch and Kelly (1959), and Walsh and Borowitz (1959), for the helium atom. In both these cases the interaction $v_i(r_i)$ is singular for small r_i, while T_{cross} in general is not; so that a solution of (3a) is a good approximation to that of (2a) in this region. We therefore expect that variational wave functions defined in this way will be rather good; and this is borne out in practice. The use of (3a) to approximate (2a) is discussed further in Section III.

In addition, two methods based on (3a) have been proposed for yielding results of rather higher accuracy. The first (Delves and Derrick 1963) generates a sequence of eigenfunctions, which are used as trial functions for (2a). These trial functions are defined in terms of the set of Sturmian eigenfunctions of the factorized one-dimensional parts of (3a). An alternative approach, suggested by Walsh and Borowitz (1959), is to carry out a perturbation expansion using (3a) as the zero-order equation. Neither of these methods has yet been tried in practice; however, the second has some difficulties in principle which arise from the form of (3a). In the next section we discuss briefly some of the properties of equation (3a) which are independent of the detailed form of the potential $v_i(r_i)$, while in Section III we discuss the possible uses of (3a) as a comparison soluble problem to (2a).

II. Properties of Separable Solutions

For simplicity we shall consider in this section the case of three identical particles of equal mass m, interacting through a pair potential $v(r)$; we shall also ignore any symmetry requirements on the wave function. Equation (3a) then becomes

$$[H_0-E]\psi(r_1,r_2,r_3) = 0, \tag{5a}$$

where

$$H_0 = \sum_i \left\{-\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial r_i^2}+\frac{2}{r_i}\frac{\partial}{\partial r_i}\right)+v(r_i)\right\}. \tag{5b}$$

The operator H_0 differs from H, equations (2), by the "perturbation" H_1,

$$H = H_0+H_1,$$

$$H_1 = \frac{\hbar^2}{m}\sum_i \frac{\mathbf{r}_j\cdot\mathbf{r}_k}{r_j r_k}\frac{\partial^2}{\partial r_j\,\partial r_k}. \tag{5c}$$

Equation (5a) has the set of separable solutions

$$\psi_{lmn} = \phi_l(r_1)\phi_m(r_2)\phi_n(r_3), \qquad E = E_{lmn} = E_l+E_m+E_n, \tag{5d}$$

where the functions $\phi_j(r)$ are solutions of the one-dimensional equations

$$\left\{-\frac{\hbar^2}{m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+v(r)-E_j\right\}\phi_j(r) = 0. \tag{6}$$

Although equation (5) is separable in this way, the complete *problem* is intrinsically not separable, since the space over which solutions of (5) are defined is not separable. Rather, r_1, r_2, r_3 are subject to the triangular inequalities

$$|r_j-r_k| \leqslant r_i \leqslant r_j+r_k. \tag{7}$$

(a) *Bound States*

Let us first look for acceptable "bound state" solutions of (5). We define a bound state to be a solution of (5) which is quadratically integrable over the space (7) with the volume element $\mathrm{d}\tau$ appropriate to equation (2a), which is

$$\mathrm{d}\tau = r_1 r_2 r_3\,\mathrm{d}r_1\,\mathrm{d}r_2\,\mathrm{d}r_3. \tag{8}$$

This definition ensures that a bound-state solution of (5) is an acceptable variational trial function for (2),† and indeed gives the variational estimate E_{V} of the eigenvalue E of (2)

$$E_{\mathrm{V}} = E_{lmn}+\frac{\int \psi_{lmn}^* H_1\,\psi_{lmn}\,\mathrm{d}\tau}{\int \psi_{lmn}^*\,\psi_{lmn}\,\mathrm{d}\tau}. \tag{9}$$

† We ignore the possibility that the numerator of (9) may diverge although the denominator does not.

For such a separable bound state to occur, we require that the potential $v(r)$ shall support a one-dimensional bound-state solution of (6); we assume here that this is the case, and that the lowest such bound state has energy E_0. In this case, we find the following completely unphysical energy spectrum of H_0:

The separable bound-state solutions of (5) form a continuum from energy $3E_0$ to ∞. (10)

The proof of (10) is simple. Let us construct a solution of (5) of (arbitrary) energy E, in the following way. We write

$$\left.\begin{aligned} E &= E_0+E_0+\epsilon, \\ \alpha^2 &= -mE_0/\hbar^2, \qquad \beta^2 = -m\epsilon/\hbar^2, \\ \psi_{\mathrm{B}} &= \phi_0(r_1)\phi_0(r_2)\phi_\epsilon(r_3). \end{aligned}\right\} \tag{11}$$

In equation (11), $\phi_0(r)$ is the ground-state solution of (6), while ϕ_ϵ is a solution of (6), regular at the origin, for $E_j = \epsilon$.

Then ψ_{B} forms a bound state if the integral $\int \psi_{\mathrm{B}}^2 \, \mathrm{d}\tau$ is finite. But the convergence of this integral is determined by the behaviour of ψ_{B} for large r_1, r_2, r_3. In this region we have in general (ϵ not an eigenvalue of (6))

$$\phi_0(r) \sim \mathrm{e}^{-\alpha r}, \qquad \phi_\epsilon(r) \sim \mathrm{e}^{+\beta r},$$

so that the dangerous direction is $r_3 \to \infty$. However, for $r_3 \to \infty$ the inequalities (7) imply

$$r_3 < r_1+r_2$$

and hence

$$\psi_{\mathrm{B}} \lesssim \exp -(\alpha-\beta)r_3. \tag{12}$$

Hence the function ψ_{B} is exponentially decreasing everywhere, and therefore forms an acceptable bound state, provided that

$$\mathrm{Re}(\alpha-\beta) > 0. \tag{12a}$$

But this is true for any energy $E > 3E_0$, since for $3E_0 < E < 2E_0$ we have $E_0 < \epsilon < 0$, and hence β is real and less than α, while for $E > 2E_0$ we have $\epsilon > 0$ and hence β is imaginary.

The reason for this behaviour is of course very simple: the operators H_0 and H_1 are not Hermitian with respect to the class of quadratically integrable functions over the space (7) with volume element (8), although $H = H_0+H_1$ is. Hence, there is no reason why the usual properties of Hermitian operators should be exhibited by H_0; in particular, it may not (and does not) have a discrete spectrum. This unphysical behaviour of H_0 does *not* matter if we are using solutions of (5) to generate trial functions for (2); however, it *does* mean that at least the usual perturbation theories cannot be applied to (5) using H_1 as a perturbation since these theories assume that both H_0 and H_1 are Hermitian, even when taken only to first order.

(b) Scattering States

A solution ψ_S of equation (2), representing the scattering of particle (3) from a bound state of particles 1 and 2 at a total energy E, has the following asymptotic form. We define ρ and k by the relations (for $m_1 = m_2 = m_3 = m$)

$$\left.\begin{aligned} \rho^2 &= \tfrac{1}{2}(r_1^2+r_2^2)-\tfrac{1}{4}r_3^2, \\ k^2 &= (4m/3\hbar^2)(E-E_0). \end{aligned}\right\} \tag{13}$$

Then for large ρ

$$\psi_S \to \phi_0(r_1)[\sin(k\rho)+\tan\delta\cos(k\rho)]/\rho. \tag{14}$$

Solutions of (5) also exist with the asymptotic form (14). The positive energy solutions of (6) have the asymptotic form for energy E:

$$\left.\begin{aligned} E &= \hbar^2 k_0^2/m, \\ \phi(E,r) &\to [\sin(k_0 r)+\tan\delta_0 k\cos(k_0 r)]/r, \end{aligned}\right\} \tag{15a}$$

while for $E = 0$ we have with a suitable normalization

$$\phi(0,r) \to 1-a_0/r^2. \tag{15b}$$

In equation (15), $\tan\delta_0$ is the phase shift of the single-particle equation (6), while a_0 is the zero-energy scattering length, for the potential $v(r)$; these are not of course directly related to the three-particle phase shift and scattering length of equation (14). Now let us choose an energy E_V and a partitioning of E_V as follows:

$$E_V \equiv 4E/3-E_0/3 = E_0+(\hbar^2/m)k^2+0. \tag{16}$$

Then the corresponding solution of (5) is

$$\begin{aligned} \psi_V &= \phi_0(r_1)\phi(\hbar^2k^2/m, r_2)\phi(0,r_3) \\ &\to \phi_0(r_1)\{[\sin(kr_2)+\tan\delta\cos(kr_2)]/r_2\}[1-a_0/r_3^2] \\ &= \phi_0(r_1)[\sin(k\rho)+\tan\delta\cos(k\rho)]/\rho+O(\rho^{-2}). \end{aligned} \tag{17}$$

Thus ψ_V has the same asymptotic form as ψ_S, equation (14), and hence may be said to represent a scattering state. We note that the energies appropriate to ψ_S and ψ_V are not the same; moreover, the convergence of ψ_V to the form (14) is rather slow. This slow convergence is *not* directly connected with the non-Hermitian character of H_0; however, it does mean that ψ_V is not a suitable trial function to use in the standard variation principles for $\tan\delta$. This point is discussed further in Delves and Derrick (1963), where it is shown that a modified variation principle for $\tan\delta$ can be derived in which ψ_V can be used.

III. A Simple Example

The previous paragraph showed that (5) is limited in usefulness as a comparison soluble problem for (2); however, it can be useful for generating bound-state variational functions, and has so been used in the fixed nucleus two-electron problem (Pluvinage 1950; Spruch and Kelly 1959; Walsh and Borowitz 1959), with $m_1 = m_2 = m$, $m_3 \to \infty$. In this case, we have (in atomic units)

$$H_0 = L_0(r_1)+L_0(r_2)+L_1(r_3), \tag{18a}$$

$$H_1 = -\frac{1}{m}\left\{\frac{r_2^2+r_3^2-r_1^2}{2r_2r_3}\frac{\partial^2}{\partial r_2\,\partial r_3}+\frac{r_3^2+r_1^2-r_2^2}{2r_3r_1}\frac{\partial^2}{\partial r_3\,\partial r_1}\right\}, \tag{18b}$$

$$H = H_0+H_1,$$

$$L_0(r) = -\tfrac{1}{2}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)-\frac{2}{r}, \tag{18c}$$

$$L_1(r) = -\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{1}{r}, \tag{18d}$$

and the variational wave function for H suggested by H_0 is

$$\psi = \phi_0(r_1)\phi_0(r_2)\phi_1(r_3), \tag{19}$$

where ϕ_0 is an eigenfunction of L_0 and ϕ_1 an eigenfunction of L_1. This wave function is expected to be a reasonable approximation if H_1 is small; and in this case it may be thought reasonable to choose ϕ_0 and ϕ_1 as the lowest-lying eigenfunctions of L_0 and L_1, satisfying the equations

$$(L_0-E_0)\phi_0(r) = 0, \tag{20a}$$

$$(L_1-E_1)\phi_1(r) = 0. \tag{20b}$$

These equations represent respectively the motions of an electron in the field of a massive nucleus of charge Z and the relative motion of two electrons in their mutual repulsive field; they therefore have well-known solutions. In fact, both Pluvinage and Walsh and Borowitz chose ψ_0 as the ground state of L_0; that is

$$\phi_0(r) = \mathrm{e}^{-Z^*r},$$

$$E_0 = -Z^{*2} \quad \text{a.u.}$$

Equation (20a) predicts $Z^* = Z$; however, of course Z^* was allowed to vary as a free parameter.

The Hamiltonian L_1 has no bound states; and Pluvinage therefore took $\phi_1(r_3)$ to be a function of positive energy E_3, E_3 being left as a variational parameter. The positive-energy solutions of (18d) are not simple; and Walsh and Borowitz, arguing as above from the assumed smallness of H_1, take $E_3 = 0$, for which the eigenfunctions are simpler. However, we saw in the previous paragraph that finiteness of ϕ_1 for large r_3 is not a necessary condition for ψ to be a satisfactory trial function for H. Rather, we obtain allowable trial functions if we take for ϕ_1 any solution of (18d) for energy $E_1 \geqslant -2Z^2$.

Further, the same argument that suggested the value $E_1 = 0$ to Walsh and Borowitz, would suggest that the value $E_1 = -2Z^2$ should be better still. We take here the wave function

$$\psi_1 = \exp \beta r_3 \exp\{-Z^*(r_1+r_2)\}. \tag{21}$$

This wave function is identical with that of Pluvinage and of Walsh and Borowitz in its r_1 and r_2 dependence; the dependence on r_3 typifies that of a negative-energy solution of (20b) (and is much simpler than that of Pluvinage or of Walsh and Borowitz).

Table 1

BOUND ON THE GROUND STATE ENERGY OF HELIUM-LIKE ION

Z	E (Pluvinage)	E (Walsh)	Eqn. (21)	Best Z^*	Best β	E (exact)
1	—	−0·498	−0·508	0·86	0·23	−0·528
2	−2·878	−2·875	−2·890	1·86	0·25	−2·904
3	−7·255	−7·249	−7·267	2·86	0·26	−7·280
4	−13·631	−13·623	−13·645	3·86	0·26	−13·656
5	−22·006	−21·997	−22·019	4·87	0·28	−22·031
6	−32·381	−32·372	−32·394	5·87	0·28	−32·406
7	−44·756	−44·746	−44·761	6·86	0·27	−44·781

The variational energies given by this wave function, on varying Z^* and β, are compared in Table 1 with those of Pluvinage and of Walsh and Borowitz. We see that, as expected (21) is somewhat better than either, although the amount of work involved in calculating the energy is much smaller.

It is also interesting to note that the prediction $E_1 = -2Z^2$ corresponds to the assignment $\beta = Z^*$ for which we find the rather poor result

$$E(Z^*, Z^*) = 0. \tag{22}$$

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V. References

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