On the three-body problem

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Abstract. We consider the ground state of a system of three interacting particles of equal mass. An integro-differential equation is obtained for the optimum pair function f in the product wavefunction $\Psi(123) = f(12)f(13)f(23)$. The solution for harmonic forces reproduces the known exact ground state. Approximate analytic solutions are obtained for inverse-square forces, and for a general force law in the semiclassical limit.

1. *Introduction.* We shall consider the ground state of a three-particle system with the Hamiltonian

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2 + \nabla_3^2) + v(12) + v(13) + v(23). \tag{1}$$

The particles are assumed to interact with pairwise, conservative and momentum-independent forces. The physical systems well represented by this Hamiltonian are the triatomic molecules of the rare gases, and (to a lesser extent) other triatomic molecules and the nuclear three-body systems, the triton and the helium three nucleus. The corrections to (1), for example, three-body forces, and spin and isospin dependent forces, appear to be small and can probably be treated as perturbations.

We shall obtain a solution to the problem of determining the ground state in the following restricted sense: considering wavefunctions of the type

$$\Psi(123) = f(12)f(13)f(23) \tag{2}$$

we determine the best f, that is, the one minimizing the expectation value of the Hamiltonian. The general solution is an implicit one, in that f is shown to satisfy a certain integro-differential equation. An explicit solution is obtained for harmonic forces, when it checks with the known exact result; approximate analytic solutions are given for two other cases. The variational method which gives the solution has previously been used to obtain equations for the ground state of a system of four or more bosons (1). The three-particle case is mathematically distinct, and is also more tractable.

The three-nucleon problem has been studied extensively (2–5), while even the existence of the lighter triatomic rare gas molecules is not yet certain (6–8). Most of the work on three-body systems has been based on the variational principle: a parametrized wavefunction of a certain type is chosen, and the expectation value of the Hamiltonian is minimized numerically by variation of the parameters. This method yields good results, but can never be completely satisfactory, because there

exists a multiple infinity of trial functions, even when one restricts the wavefunction to be of a given form (e.g. the symmetric product of equation (2)). We shall derive an equation for the best pair function f which can be solved numerically. Analytic solutions are obtained in certain special cases.

2. *The variational equation.* The derivation of the equation to be satisfied by the best pair function f for the three-body system is similar to that for the N-boson system (1). We shall therefore abbreviate the discussion.

The expectation value of the Hamiltonian is $\mathscr{E}/\mathscr{I}$, where

$$\mathscr{E} = \int d1\,d2\,d3\,\Psi H\Psi,$$

$$\mathscr{I} = \int d1\,d2\,d3\,\Psi^2. \tag{3}$$

To keep the notation of reference (1) we shall work in terms of density correlation functions defined by

$$\mathscr{I}n(1\ldots s) = \frac{N!}{(N-s)!}\int d(s+1)\ldots dN\,\Psi^2 \tag{4}$$

where $N = 3$ and $s = 1, 2$ or 3. It is convenient to write Ψ as

$$\Psi(123) = \exp\{\tfrac{1}{2}(\phi(12)+\phi(13)+\phi(23))\}. \tag{5}$$

The expectation value of the Hamiltonian then becomes

$$\mathscr{E}/\mathscr{I} = \frac{1}{2}\int d1\,d2\,n(12)\left[-\frac{\hbar^2}{8m}(\nabla_1^2+\nabla_2^2)\,\phi(12)+v(12)\right]. \tag{6}$$

The best ϕ is determined by the variational condition $\delta(\mathscr{E}/\mathscr{I}) = 0$; taking variations $\delta\phi$ in ϕ, we obtain the equation

$$\int d1\,d2\{\delta n(12)\,[(\nabla_1^2+\nabla_2^2)\,\phi(12) - 8mv(12)/\hbar^2] + \delta\phi(12)\,(\nabla_1^2+\nabla_2^2)\,n(12)\} = 0. \tag{7}$$

The variation $\delta n(12)$ in the pair density function is found from the defining equation (cf. eq. (17) of (1)):

$$\delta n(12) = (\delta\phi(12)-\delta\mathscr{I}/\mathscr{I})\,n(12)+\int d3(\delta\phi(13)+\delta\phi(23))\,n(123). \tag{8}$$

Equations (7) and (8), and the fact that the density correlation functions are completely symmetric, then lead to the variational equation

$$[\lambda+\theta(12)+\nabla_1^2+\nabla_2^2]\,n(12)+\int d3[\theta(13)+\theta(23)]\,n(123) = 0, \tag{9}$$

where

$$\lambda = \frac{8m}{\hbar^2}\,(\mathscr{E}/\mathscr{I}) \tag{10}$$

and

$$\theta(12) = (\nabla_1^2+\nabla_2^2)\,\phi(12) - 8mv(12)/\hbar^2. \tag{11}$$

The equation corresponding to (9) for the N-boson problem contains the additional term

$$\tfrac{1}{2}\int d3\,d4\,\theta(34)\,n(1234).$$

The Laplacian of the pair density function can be expressed in terms of derivatives of ϕ. We have

$$\nabla_1 n(12) = n(12)\,\nabla_1\phi(12)+\int d3n(123)\,\nabla_1\phi(13) \tag{12}$$

and

$$\nabla_1 n(123) = n(123)\,[\nabla_1\phi(12)+\nabla_1\phi(13)]. \tag{13}$$

Therefore

$$\nabla_1^2 n(12) = n(12) \left[\nabla_1^2 \phi(12) + (\nabla_1 \phi(12))^2 \right] + \int d3 n(123) \left[\nabla_1^2 \phi(13) + 2\nabla_1 \phi(12) . \nabla_1 \phi(13) + (\nabla_1 \phi(13))^2 \right]. \quad (14)$$

Substituting in (9), we obtain the equation

$$n(12) \left[\lambda + 2(\nabla_1^2 + \nabla_2^2) \phi(12) + (\nabla_1 \phi(12))^2 + (\nabla_2 \phi(12))^2 - 8mv(12)/\hbar^2 \right]$$
$$+ 2\int d3 n(123) \left[(2\nabla_1^2 + \nabla_3^2) \phi(13) + (\nabla_1 \phi(13))^2 + 2\nabla_1 \phi(12) . \nabla_1 \phi(13) - 8mv(13)/\hbar^2 \right] = 0. \quad (15)$$

Since

$$\frac{n(123)}{n(12)} = \frac{\exp[\phi(13) + \phi(23)]}{\int d3 \exp[\phi(13) + \phi(23)]}, \quad (16)$$

we have the best ϕ determined as the solution of an integro-differential equation. If we further assume that $v(12)$ and $\phi(12)$ are functions of r_{12} only, we can carry out the integration over the azimuthal angle, and the equation reduces to

$$\left[\lambda + \frac{4}{r}(r\phi(r))'' + 2(\phi'(r))^2 - \frac{8mv(r)}{\hbar^2} \right] \int_0^\infty ds\, s e^{\phi(s)} \int_{|r-s|}^{r+s} dt\, t\, e^{\phi(t)} + 2\int_0^\infty ds\, s e^{\phi(s)} \int_{|r-s|}^{r+s} dt\, t\, e^{\phi(t)}$$
$$\times \left[\frac{3}{s}(s\phi(s))'' + \frac{r^2 + s^2 - t^2}{rs} \phi'(r)\, \phi'(s) + (\phi'(s))^2 - \frac{8mv(s)}{\hbar^2} \right] = 0. \quad (17)$$

3. *Harmonic forces.* The three-body Schrödinger equation for particles of equal mass interacting with harmonic forces can be solved exactly (9, 10), and the ground state wavefunction is of the product form. Thus our equation should give the exact results. We shall check that it does. We set $\phi = -(r/a)^2$, and use the dimensionless variables

$$x = \frac{r}{a}, \quad \epsilon = \frac{2ma^2}{\hbar^2} (\mathscr{E}/\mathscr{I}), \quad u = \frac{2ma^2}{\hbar^2} v. \quad (18)$$

Equation (17) becomes

$$[\epsilon - 15 + 4x^2 - u(x)] \int_0^\infty dy\, y\, e^{-y^2} \int_{|x-y|}^{x+y} dz\, z\, e^{-z^2} + 2\int_0^\infty dy\, y\, e^{-y^2} \int_{|x-y|}^{x+y} dz\, z\, e^{-z^2}[y^2 - u(y)] = 0. \quad (19)$$

We look for a solution of the form $u(x) = u(0) + \gamma x^2$. The integrals in (19) may be derived from the basic integral

$$\int_0^\infty dy\, y\, e^{-\alpha y^2} \int_{|x-y|}^{x+y} dz\, z\, e^{-\beta z^2} = \tfrac{1}{2}\pi^{\frac{1}{2}}(\alpha+\beta)^{-\frac{3}{2}} x \exp\left\{ -\left(\frac{\alpha\beta}{\alpha+\beta}\right) x^2 \right\}. \quad (20)$$

We find that the harmonic potential does satisfy (19) for $\gamma = 3$. The eigenvalue is $\epsilon = 3(u(0) + 6)$. We have thus shown that the function

$$\Psi(123) = \exp\left\{ -(r_{12}^2 + r_{13}^2 + r_{23}^2)/2a^2 \right\} \quad (21)$$

is the optimum wavefunction of the product type for the pair potential

$$v(r) = v(0) + \frac{3\hbar^2}{2ma^2}\left(\frac{r}{a}\right)^2. \quad (22)$$

Its energy is

$$E = 3\left\{ v(0) + \frac{3\hbar^2}{ma^2} \right\}. \quad (23)$$

These results coincide with those of reference (10).

4. *Inverse-square law forces.* The method of the last section indicates a possible path to further analytic solutions, namely to consider the inverse problem: given ϕ, to find the potential for which this ϕ is the solution of our variational equation. Instead of a non-linear integro-differential equation for ϕ, we then have to solve a linear integral equation for v.

The simplest ϕ, apart from that of the previous section, is $\phi = -r/a$, i.e.

$$\Psi(123) = \exp\left\{-(r_{12}+r_{13}+r_{23})/2a\right\}. \tag{24}$$

This wavefunction is of historical interest, since it was used (with a as a variational parameter) in the earliest calculations of the ground state energy of the triton (2). We shall find that the wavefunction (24) is, to a very good approximation, the optimum wavefunction for a r^{-1} potential.

We set $\phi = -r/a$ in (17) and use the dimensionless variables defined in (18). Equation (17) reduces to

$$\left[\epsilon + 1 - \frac{2}{x} - u(x)\right]\int_0^\infty dy\, y\, e^{-y}\int_{|x-y|}^{x+y} dz\, z\, e^{-z}$$
$$+ \int_0^\infty dy\, y\, e^{-y}\int_{|x-y|}^{x+y} dz\, z\, e^{-z}\left[\frac{x^2+y^2-z^2}{2xy} - \frac{3}{y} - 2u(y)\right] = 0. \tag{25}$$

The potential $u(x)$ is singular at the origin: $u \sim -2/x$. We therefore set

$$u(x) = -2/x + w(x).$$

In the resulting equation for w, the integrals not involving w may be derived from the basic integral

$$\int_0^\infty dy\, e^{-\alpha y}\int_{|x-y|}^{x+y} dz\, e^{-\beta z} = 2\frac{e^{-\beta x}-e^{-\alpha x}}{\alpha^2-\beta^2}. \tag{26}$$

We find that w satisfies the Fredholm integral equation

$$[1 + x + \tfrac{1}{3}x^2]\, w(x) + 4\int_0^\infty dy\, K(x,y)\, w(y) = (\epsilon+2) + (\epsilon+\tfrac{7}{3})\, x + \tfrac{1}{3}(\epsilon+2)\, x^2, \tag{27}$$

where

$$K(x,y) = \frac{y}{x}e^{x-y}\int_{|x-y|}^{x+y} dz\, z\, e^{-z}. \tag{28}$$

We require w to go to zero at infinity at least as fast as $1/x$. We set $w(x) \sim c/x$ and calculate the dominant terms in (27) for large x. The only term in x^2 is the last, which determines the eigenvalue: $\epsilon = -2$. The terms in x give $c = \tfrac{1}{7}$. At the origin, w is regular. We find

$$\left.\begin{aligned} w(0) &= -8\int_0^\infty dx\, x^2\, e^{-2x}w(x),\\ w'(0) &= \tfrac{1}{3}. \end{aligned}\right\} \tag{29}$$

The first relation implies that $w(x)$ changes sign at least once. Numerical solution of equation (27) with $\epsilon = -2$ shows that w rises from a value of approximately $-0{\cdot}09$ at the origin to a maximum of about $0{\cdot}06$ at $x \simeq 1{\cdot}65$, and then decreases monotonically. Thus w is always small in comparison to $2/x$, the maximum ratio being attained asymptotically.

We have thus shown that, to an accuracy of seven per cent in the potential, the function of equation (24) is the optimum wavefunction of the product type for the pair potential

$$v(r) = -\left(\frac{\hbar^2}{ma}\right) r^{-1} \tag{30}$$

with energy

$$E = -\frac{\hbar^2}{ma^2}. \tag{31}$$

5. *A semiclassical approximation.* Finally, we shall give an approximate solution of the equation for the pair function in the semiclassical case where the three bodies are strongly localized near their equilibrium positions. We thus obtain a correction to the classical binding energy.

Let the pair function have a strong maximum at $r = b$. The first two terms of a Taylor expansion of ϕ about $r = b$ give $\phi = \text{constant} - (r-b)^2/a^2$. If the maximum is nearly symmetric about $r = b$, the next term $(r-b)^3$ will have a small coefficient. Then using the notation of equation (18) and with $\xi = b/a$, (17) reduces to

$$\int_0^\infty dy\, y\, e^{-(y-\xi)^2} \int_{|x-y|}^{x+y} dz\, z\, e^{-(z-\xi)^2} \left\{ \epsilon - 15 + \frac{4\xi}{x} + 2(x-\xi)^2 - u(x) \right.$$
$$\left. + 2\left[\frac{3\xi}{y} + \frac{x^2+y^2-z^2}{xy}(x-\xi)(y-\xi) + (y-\xi)^2 - u(y) \right] \right\} = 0. \tag{32}$$

For $x < 2\xi$, the dominant contribution to the integrals in (32) comes from the region around $y = \xi = z$. A first approximation to the solution is thus obtained by putting y and z equal to ξ in the integrand. This gives the relation

$$\epsilon - 5 - 4(x-\xi)/x + 2(x-\xi)^2 - u(x) - 2u(\xi) = 0. \tag{33}$$

Thus, to this approximation, the appropriate potential is

$$u(x) = u(\xi) - 4(x-\xi)/x + 2(x-\xi)^2, \tag{34}$$

and the corresponding eigenvalue is $\epsilon = 3u(\xi) + 5$. If the wavefunction is to be well localized near $r = b$, we need a much less than b, i.e. large ξ. The minimum of $u(x)$ is at $x = \xi + \xi^{-1} + O(\xi^{-2})$ and is $u_0 = u(\xi) + O(\xi^{-2})$. The second derivative of u at its minimum is equal to four. Thus we have shown that, neglecting terms smaller by the factor $(a/b)^2$,

$$\Psi(123) = \exp\left\{ -[(r_{12}-b)^2 + (r_{13}-b)^2 + (r_{23}-b)^2]/2a^2 \right\} \tag{35}$$

is an optimum wavefunction for pair potentials $v(r)$ with minimum v_0 and second derivative $2\hbar^2/ma^2$ at $r = b$. The ground state energy is

$$E = 3\left\{ v_0 + \frac{5\hbar^2}{6ma^2} \right\}. \tag{36}$$

This formula gives the quantum correction to the classical energy $3v_0$ when there is strong binding, e.g. for the heavier triatomic molecules of the rare gases. For example, in the case of the 6–12 potential

$$v(r) = v_0 \left\{ 2\left(\frac{b}{r}\right)^6 - \left(\frac{b}{r}\right)^{12} \right\}, \tag{37}$$

equation (36) gives the energy

$$E = 3\left\{v_0 + 5\left(\frac{\hbar^2|v_0|}{mb^2}\right)^{\frac{1}{2}}\right\}. \tag{38}$$

The second term is about forty per cent of the first for neon, and becomes progressively smaller for the heavier rare gases. Unfortunately, the formulae derived in this section are not applicable to the triton or to triatomic molecules of helium. These are weakly bound (relative to $3v_0$) and thus cannot be sharply localized.

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