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# Three-body S-state wavefunctions: symmetry and degrees of freedom associated with normalisation of the exact wavefunction

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**Abstract.** The few-particle Schrödinger equation does not define the symmetry of the wavefunction, which must be chosen to match the symmetry of the particles. It is shown, by reference to the S-states of a three-particle system, that the symmetry does constrain degrees of freedom associated with normalisation of the exact wavefunction. The first particle is treated as infinitely massive, and distinguishable. The systems where the second and third particles are (i) distinguishable, (ii) indistinguishable with a symmetric wavefunction (bosons) and (iii) indistinguishable with an antisymmetric wavefunction (fermions) may be treated as special cases of a continuous description of particle symmetry. Cases (ii) and (iii) are opposite extremes in the analysis.

## 1. Introduction

In recent years there has been increased interest in solving the Schrödinger equation for few-body systems exactly, using spherical polar coordinates (Newman 1973, Davis and Maslen 1982a, b, 1983a, b). Substitution of a series of sufficiently general form into the equation yields recurrence equations relating coefficients which, when determined, specify the wavefunction completely.

Although few-particle systems have been studied successfully in interparticle coordinates (Hylleraas 1929) and in hyperspherical coordinates (Haftel and Mandelzweig 1983), spherical polar coordinates have some advantages. The recurrence equations derived from the Schrödinger equation using spherical polar coordinates are simpler than that obtained using interparticle distances. The asymptotic form of the wavefunction is established more easily than that for hyperspherical coordinates. For example the form of an atomic wavefunction in the asymptotic limit of one electron being an infinite distance from the nucleus is not obvious in hyperspherical coordinates.

In spherical polars simplification of at least the low-order coefficients has been achieved for the ground state of helium (Davis and Maslen 1983a). A compact form for the exact wavefunction will be obtained if that simplification can be extended to the higher-order coefficients.

A power series in  $r_1$  and  $r_2$  does not yield physically acceptable solutions. Logarithmic terms must be introduced (White and Stillinger 1970, Morgan 1978, Haftel and Mandelzweig 1983). It is convenient to use a solution with different analytical forms in the regions  $r_1 > r_2$  and  $r_1 < r_2$ .

The solution must be normalisable and must belong to the domain on which the Hamiltonian operator is Hermitian. This Hermiticity condition requires continuity of the function and the first derivatives at the boundary  $r_1 = r_2$  (Davis and Maslen 1982b). The lowest-order coefficients derived from the recurrence relation and the boundary conditions provide a starting point from which most of the remaining coefficients can be evaluated. The energy eigenvalues and the remaining coefficients are determined by the requirements for the normalisability of the wavefunction.

The three-particle system where two of the particles interact with the third but not with each other is a special case of the general three-particle system. This case is easily solved as the wavefunction can be expressed as a product of two two-particle wavefunctions.

A system of particular interest is a pair of identical particles in the field of a third where all particles interact with each other. There are two distinct cases, described by symmetric or antisymmetric wavefunctions, corresponding to bosons and fermions respectively (Schiff 1968, p 42).

These special cases of the general three-particle system are often treated separately. The work below describes a unified treatment up to the point of applying the normalisability condition.

Although the Schrödinger equation does not depend on particle symmetry for its validity, it is shown below that the terms to be evaluated using the normalisability condition vary with the symmetry of the wavefunction. This is at first surprising as there is no obvious linking of the square-integrability and Hermiticity conditions with the symmetry of the formal solution.

## 2. Equations for three non-identical particles

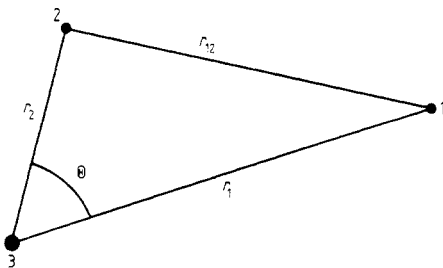
The S-state wavefunctions can be chosen to be functions of the coordinates  $r_1$ ,  $r_2$  and  $\Omega = \cos \Theta$  as shown in figure 1.

For convenience it is assumed particles 1 and 2 have identical mass and the third particle has infinite mass. Particles 1 and 2 are distinguishable if the 1-3 and 2-3 interparticle potentials are different. The Hamiltonian in the Schrödinger equation

$$H\Psi(r_1, r_2, \Omega) = E\Psi(r_1, r_2, \Omega) \quad (1)$$

may be written

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + V(r_1, r_2, \Omega) \quad (2)$$



**Figure 1.** Coordinates for describing the S-states of a three-particle system where particle 3 is massive.

where  $V$  is comprised of three interparticle potential terms. These are not stated explicitly but are contained in  $V(r_1, r_2, \Omega)$  so as to keep the nature of the interparticle potentials general. For the coordinates  $r_1, r_2, \Omega$  the Hamiltonian becomes

$$-\frac{1}{2} \left[ r_1^{-2} \frac{\partial}{\partial r_1} \left( r_1^2 \frac{\partial}{\partial r_1} \right) + r_2^{-2} \frac{\partial}{\partial r_2} \left( r_2^2 \frac{\partial}{\partial r_2} \right) + (r_1^{-2} + r_2^{-2}) \frac{\partial}{\partial \Omega} \left( (1 - \Omega^2) \frac{\partial}{\partial \Omega} \right) \right] + V(r_1, r_2, \Omega).$$

As the Legendre polynomials  $P_l(\Omega)$  (Abramowitz and Stegun 1965) are eigenfunctions of the differential operator, that is,

$$\frac{\partial}{\partial \Omega} \left( (1 - \Omega^2) \frac{\partial}{\partial \Omega} \right) P_l(\Omega) = -l(l+1) P_l(\Omega)$$

it is natural to use a multipole expansion of the wavefunction. The expansion is similar to that described and justified by Davis and Maslen (1982b),

$$\Psi(r_1, r_2, \Omega) = \begin{cases} \exp(-\lambda_1 r_1 - \lambda_2 r_2) \sum_{ijlp} C_{ijlp} r_1^j r_2^l [e^{qr_1} \text{Ei}(-qr_1)]^p P_l(\Omega) / p! & r_1 > r_2 \\ \exp(-\lambda_1 r_2 - \lambda_2 r_1) \sum_{ijlp} C'_{ijlp} r_1^j r_2^l [e^{qr_2} \text{Ei}(-qr_2)]^p P_l(\Omega) / p!; & r_1 < r_2 \end{cases} \quad (3)$$

where  $l, p, q \geq 0$ . For square-integrability at the origin non-zero coefficients are restricted to

$$i + j \geq -1. \quad (4)$$

$\text{Ei}(x)$  is the exponential integral (Abramowitz and Stegun 1965). The term in square brackets may be expressed as the sum of a log function and a power series with a form that depends on  $q$ . Parameter  $q$  may be chosen to optimise the convergence of the coefficients  $C_{ijlp}$  and  $C'_{ijlp}$ . Parameters  $\lambda_1$  and  $\lambda_2$  are chosen so that the exponential terms in (3) match the asymptotic behaviour of the wavefunction. The inclusion of logarithmic terms provides the flexibility required for derivative continuity at the boundary  $r_1 = r_2$  (Davis and Maslen 1982b). Inclusion of Legendre functions of the second kind,  $Q_l(\Omega)$ , in the expansion is forbidden by the requirement that eigenfunctions of the Hamiltonian (2) belong to the domain for which it is Hermitian. The expression for  $\Psi(r_1, r_2, \Omega)$  belongs to that domain, and also satisfies the requirement of local square-integrability at the origin.

Davis and Maslen (1982b) obtained numerical estimates of the coefficients of the series for the ground state of helium. They found that successive coefficients of the series in  $r_1$  and  $r_2$  decrease by approximately one order of magnitude. Although the series in  $P_l(\Omega)$  converges less rapidly, the smooth variation of the coefficients with  $l$  for large  $l$  suggests the possibility, eventually, of summing analytically over this index.

### 2.1. Solution of the differential equations

Substituting the function (3) into equation (1) provides two recurrence equations which relate the coefficients  $C_{ijlp}$  and  $C'_{ijlp}$  within each of the series. The recurrence equations do not specify all the coefficients completely. The solution must be completed by applying the boundary conditions.

Hermiticity requires continuity of the function and its first derivatives at  $r_1 = r_2$  (Davis and Maslen 1982b). Satisfying the normalisability condition requires an examination of the asymptotic form of the coefficients, some of which are necessarily

undetermined during the initial calculation. Normalisability also determines the energy eigenvalues.

If the formal series (3) had included all positive and negative powers of  $r_1$  and  $r_2$ , it would be impossible to choose an initial group of coefficients from which the recurrence equation could specify the remainder. However the square-integrability and Hermiticity conditions restrict the allowed powers of  $r_1$  and  $r_2$  to a semi-infinite region. The lowest order coefficients in this region are determined by the recurrence and derivative continuity equations, providing a natural starting point for calculating the remaining coefficients.

The recurrence equation obtained for  $C_{ijlp}$  by substituting the trial series (3) into the Schrödinger equation is

$$\begin{aligned} & \{l, i + 2\}C_{i+2jlp} + \{l, j + 2\}C_{ij+2lp} \\ &= -(i + 2)(\lambda_1 - qp)C_{i+1jlp} - \lambda_2(j + 2)C_{ij+1lp} + (2i + 5)/2C_{i+2jlp+1} \\ &+ [q(p + \frac{1}{2}) - \lambda_1]C_{i+1jlp+1} + \frac{1}{2}C_{i+2jlp+2} \\ &+ (E + \frac{1}{2}\lambda_1^2 + \frac{1}{2}\lambda_2^2 + \frac{1}{2}p^2q^2 - \lambda_1pq - V_{op})C_{ijlp} \end{aligned} \tag{5}$$

where  $\{a, b\} = [a(a + 1) - b(b + 1)]/2$ . The effect of the potential term in the Hamiltonian,  $V(r_1, r_2, \Omega)$  is represented by  $V_{op}C_{ijlp}$ . The recurrence equation for  $C'_{ijlp}$  is identical to (5) with the 1-3 and 2-3 potentials in  $V_{op}$  interchanged.

The Hermiticity condition restricts non-zero  $C_{ijlp}$  and  $C'_{ijlp}$  to the region (Davis and Maslen 1982b)

$$j \geq 0. \tag{6}$$

The artificial boundary due to the different analytical forms of  $\Psi$  in the regions  $r_1 > r_2$  and  $r_1 < r_2$  further restricts the coefficients. The Hermiticity condition requires the wavefunction,  $\Psi$ , and its first derivatives  $\partial\Psi/\partial r_1$ ,  $\partial\Psi/\partial r_2$  to be continuous at the boundary  $r_1 = r_2$ .

Applying the three continuity conditions yields equations relating  $C_{ijlp}$  to  $C'_{ijlp}$ . Using the restrictions (4) and (6) the coefficients may be derived systematically.

Continuity of  $\Psi$  requires that

$$\sum_k (C_{ijlp} - C'_{ijlp}) = 0 \tag{7}$$

where  $\Sigma_k$  is shorthand for  $\Sigma_{i,j: i+j=k}$ . Continuity of the derivatives requires that

$$\sum_k (iC_{ijlp} - jC'_{ijlp}) = -D(k, l, p) \tag{8}$$

and

$$\sum_k (iC'_{ijlp} - jC_{ijlp}) = -D'(k, l, p) \tag{9}$$

where

$$D(k, l, p) = \sum_k C_{ijlp+1} + pq \sum_{k-1} C_{ijlp} - \sum_{k-1} (\lambda_1 C_{ijlp} - \lambda_2 C'_{ijlp})$$

and

$$D'(k, l, p) = \sum_k C'_{ijlp+1} + pq \sum_{k-1} C'_{ijlp} - \sum_{k-1} (\lambda_1 C'_{ijlp} - \lambda_2 C_{ijlp}).$$

All coefficients with  $j < l$  are proportional to other coefficients with smaller values of  $j$ . When restriction (6) is applied all  $C_{ijl}$  with  $j < l$  vanish.  $C_{ill}$  is independent of the coefficients with lower  $j$  and is not required to be zero. Therefore applying restriction (6) to the recurrence equation requires non-zero  $C_{ijl}$  and  $C'_{ijl}$  to have

$$j \geq l. \quad (10)$$

By a similar argument restriction (4) requires non-zero  $C_{ijl}$  and  $C'_{ijl}$  to have

$$i + j \geq 0. \quad (11)$$

The coefficients are calculated using a procedure similar to that described by Davis and Maslen (1982b) for the restricted case of symmetric S-states. This applies for any potential  $V$  which is not as singular as  $r_1^{-2}$  or  $r_2^{-2}$  at the origin. Writing recurrence equation (5) in the shorthand form

$$\{l, i' + 2\}C_{i'+2j'l} + \{l, j' + 2\}C_{i'j'+2lp} = -R(k, l, g, p) \quad (12)$$

(where  $k = i + j = i' + j' + 2$  and  $g = j' - l + 2$ ), the coefficients on the left-hand side belong to the line  $i + j = k$ . Similarly

$$\{l, i' + 2\}C'_{i'+2j'l} + \{l, j' + 2\}C'_{i'j'+2lp} = -R'(k, l, g, p). \quad (13)$$

Because  $V$  is not as singular as  $r_1^{-2}$  or  $r_2^{-2}$  at the origin the functions  $R(k, l, g, p)$  and  $R'(k, l, g, p)$  contain only coefficients with higher values of  $p$  or lower values of  $k$ . These are already known.

Likewise functions  $D(k, l, p)$  and  $D'(k, l, p)$  in the derivative continuity equations (8) and (9) contain known coefficients with higher values of  $p$  or lower values of  $k$ .

Using recurrence equations (12) and (13) all  $C_{ijl}$  with  $j > l$  can be written in terms of  $C_{k-llp}$  and  $R(k, l, g, p)$ , and all  $C'_{ijl}$  with  $j > l$  can be written in terms of  $C'_{k-llp}$  and  $R'(k, l, g, p)$ . The continuity equation (7) becomes

$$(C_{k-llp} - C'_{k-llp})W(k, l, 0) = 2 \sum_{g=1}^{\infty} \frac{W(k, l, g)}{g(2l+g+1)} [R'(k, l, g, p) - R(k, l, g, p)] \quad (14)$$

where

$$W(k, l, g) = \frac{1}{2} {}_3F_2(1, k/2 + 3/2, g/2 + l/2 - k/4; g/2 + 1, l + g/2 + 3/2; 1)$$

is a generalised hypergeometric function (Bailey 1935).

Equations (8) and (9) yield

$$\begin{aligned} & Y(k, l, 0)C_{k-llp} + Z(k, l, 0)C'_{k-llp} \\ &= -2 \sum_{g=1}^{\infty} g^{-1}(2l+g+1)^{-1} [Y(k, l, g)R(k, l, g, p) \\ & \quad + Z(k, l, g)R'(k, l, g, p)] - D(k, l, p) \end{aligned} \quad (15)$$

and

$$\begin{aligned} & Z(k, l, 0)C_{k-llp} + Y(k, l, 0)C'_{k-llp} \\ &= -2 \sum_{g=1}^{\infty} g^{-1}(2l+g+1)^{-1} [Z(k, l, g)R(k, l, g, p) \\ & \quad + Y(k, l, g)R'(k, l, g, p)] - D'(k, l, p) \end{aligned} \quad (16)$$

where

$$Y(k, l, g) = \frac{1}{2}[X(k, l, g) + kW(k, l, g)]$$

$$Z(k, l, g) = \frac{1}{2}[X(k, l, g) - kW(k, l, g)].$$

$$X(k, l, g) = (k/2 - g - l + 1) {}_3F_2(1, k/2 + 3/2, g/2 \\ + l/2 - k/4 + 1/2; g/2 + 1, l + g/2 + 3/2; 1)$$

is equivalent to the function reduced by Davis and Maslen (1983a). Equations (14), (15) and (16) are linear dependent and equations (15) and (16) are sufficient to calculate  $C_{k-llp}$  and  $C'_{k-llp}$  as long as the determinant

$$Y^2(k, l, 0) - Z^2(k, l, 0) \neq 0$$

that is

$$kX(k, l, 0)W(k, l, 0) \neq 0. \quad (17)$$

Once these coefficients have been calculated the remaining coefficients in the line  $i + j = k$  are determined by the recurrence equations.

Functions  $X(k, l, g)$  and  $W(k, l, g)$  are derived from the kinetic energy operator of the Hamiltonian (2) and are thus independent of the potential.

## 2.2. The degrees of freedom

The degrees of freedom provided by the coefficients  $C_{k-llp}$  and  $C'_{k-llp}$  enable the continuity and derivative continuity equations to be satisfied for a non-zero determinant (17). When the determinant is zero equations (15) and (16) cannot be used to calculate  $C_{k-llp}$  and  $C'_{k-llp}$ . The degree of freedom required by the continuity and derivative continuity equations is then provided by  $C_{k-llp+1}$  and  $C'_{k-llp+1}$ . As  $R(k, l, g, p)$  and  $R'(k, l, g, p)$  contain coefficients with higher values of  $p$ , the  $p = P + 1$  coefficients are used to satisfy the  $p = P$  equations. This is possible (i) because there is a maximum value of  $p$  ( $p_{\max}$ ) where any coefficients with  $p > p_{\max}$  are zero, and (ii) because the  $p = P + 1$  equations do not determine the  $p = P + 1$  coefficients entirely when  $k = 2l + 2n$ .

At this stage some  $p = 0$  coefficients remain to be determined. The derivative continuity condition is satisfied for arbitrary values of these coefficients, so these are referred to as 'arbitrary coefficients'. These are completely specified by the requirement that the wavefunction be normalisable (Davis and Maslen 1983b).

To calculate when the determinant (17) vanishes,  $X(k, l, 0)$  and  $W(k, l, 0)$  may be written in hypergeometric form

$$X(k, l, 0) = (k/2 - l + 1) {}_2F_1(k/2 + 3/2, l/2 - k/4 + 1/2; l + 3/2; 1)$$

$$W(k, l, 0) = \frac{1}{2} {}_2F_1(k/2 + 3/2, l/2 - k/4; l + 3/2; 1),$$

and simplified using standard formulae (Abramowitz and Stegun 1965) to

$$X(k, l, 0) = \frac{-\Gamma(l + 3/2)2^{2+k/2-l}\pi^{1/2}}{\Gamma(l/2 + k/4 + 1)\Gamma(l/2 - k/4)} \\ W(k, l, 0) = \frac{\Gamma(l + 3/2)2^{k/2-l}\pi^{1/2}}{\Gamma(l/2 + k/4 + 3/2)\Gamma(l/2 - k/4 + 1/2)}. \quad (18)$$

$X(k, l, 0)$  vanishes whenever  $k = 2l + 4n$ ;  $n = 0, 1, 2, \dots$  whereas  $W(k, l, 0)$  vanishes

whenever  $k = 2l + 4n + 2$ ;  $n = 0, 1, 2, \dots$  that is the determinant vanishes when  $k = 0, 2l + 2n$ .

The coefficients  $C_{k-3lp}$  and  $C'_{k-3lp}$  with  $p > 0$  must have values which satisfy the continuity and derivative continuity equations for  $k = 0, 2l + 2n$ . For  $k = 0, 2l + 2n$  the only coefficients left undetermined are  $C_{k-3l0}$ .

For  $k = 2l + 4n + 2$  the equations determining  $C_{k-3lp+1}$  and  $C'_{k-3lp+1}$  may be summarised as

$$\sum_{g=1}^{\infty} \frac{W(k, l, g)}{g(2l+g+1)} [R(k, l, g, p) - R'(k, l, g, p)] = 0 \quad (19)$$

and

$$\begin{aligned} X(k, l, 0)(C_{k-3lp+1} + C'_{k-3lp+1}) \\ = -2 \sum_{g=1}^{\infty} \frac{X(k, l, g)}{g(2l+g+1)} [R(k, l, g, p+1) + R'(k, l, g, p+1)] - 2D(k, l, p+1). \end{aligned} \quad (20)$$

The order of solution is that of decreasing  $p$ , starting from the maximum value,  $p_{\max}$ , which increases by one at  $k = 2l + 4n + 2$ ,  $n = 0, 1, 2, \dots$ . All  $C_{k-3lp}$  and  $C'_{k-3lp}$  are determined unless  $p = 0$ . Putting  $p + 1 = 0$  in equation (20) gives a value for  $C_{k-3l0} + C'_{k-3l0}$ . Similarly  $p_{\max}$  increases by one for  $k = 2l + 4n$ , and the equations determining  $C_{k-3lp+1}$  and  $C'_{k-3lp+1}$  are

$$\sum_{g=1}^{\infty} \frac{X(k, l, g)}{g(2l+g+1)} [R(k, l, g, p) + R'(k, l, g, p)] + D(k, l, p) = 0 \quad (21)$$

and

$$\begin{aligned} W(k, l, 0)(C_{k-3lp+1} - C'_{k-3lp+1}) \\ = -2 \sum_{g=1}^{\infty} \frac{W(k, l, g)}{g(2l+g+1)} [R(k, l, g, p+1) - R'(k, l, g, p+1)]. \end{aligned} \quad (22)$$

Putting  $p + 1 = 0$  determines  $C_{k-3l0} - C'_{k-3l0}$ .

The determinant (17) also vanished for all  $l$  when  $k = 0$ , suggesting the existence of arbitrary coefficients for all  $l$ . Examination of the continuity and derivative continuity equations shows that  $C_{-3l0} = C'_{-3l0} = 0$  for  $l > 0$  and

$$C_{0000} = C'_{0000} \quad (23)$$

is the only arbitrary coefficient with  $k = 0$ . The values of  $C_{k-3l0}$ ,  $k = 2l + 2n$ ;  $n = 0, 1, 2, \dots$  are determined by the requirement of a normalisable wavefunction (Davis and Maslen 1982b, 1983b). The special case of  $C_{0000}$  is evaluated by equating the norm of the wavefunction to unity.

### 3. The symmetric case

Consider a symmetric wavefunction

$$\Psi(r_1, r_2, \Omega) = \begin{cases} \exp(-\lambda_1 r_1 - \lambda_2 r_2) \sum_{ijlp} C_{ijlp} r_1^i r_2^j [e^{qr_1} \text{Ei}(-qr_1)]^p P_l(\Omega) / p! & r_1 > r_2 \\ \exp(-\lambda_1 r_2 - \lambda_2 r_1) \sum_{ijlp} C_{ijlp} r_1^j r_2^i [e^{qr_2} \text{Ei}(-qr_2)]^p P_l(\Omega) / p! & r_1 < r_2. \end{cases} \quad (24)$$



This is identical to the series for the general three-particle equation (3) when

$$C_{ijlp} = C'_{ijlp}. \quad (25)$$

The recurrence equation is identical to (5). Continuity is conferred by the symmetry. Derivative continuity requires

$$\sum_k (i-j) C_{ijlp} = - \sum_k C_{ijlp+1} - pq \sum_{k-1} C_{ijlp} + (\lambda_1 - \lambda_2) \sum_{k-1} C_{ijlp} = -D(k, l, p).$$

Function  $D(k, l, p)$  is similar to that used in the general three-particle equations. Non-zero coefficients are restricted to the same region of the  $ij$  plane as for three non-identical particles (10, 11). The method of solution of the equations is identical.

The equation

$$X(k, l, 0) C_{k-llp} = -2 \sum_{g=1}^{\infty} \frac{X(k, l, g)}{g(2l+g+1)} R(k, l, g, p) - D(k, l, p) \quad (26)$$

determines the  $g=0$  coefficient.

Arbitrary coefficients arise whenever  $X(k, l, 0) = 0$ . The expression for  $X(k, l, 0)$ , equation (18), shows this occurs whenever  $k = 2l + 4n$ ,  $n = 0, 1, 2, \dots$ . Therefore the first arbitrary coefficient, to be evaluated by setting the norm equal to unity, occurs at  $k=0$ . The infinite series (24) starts at  $k=0$  and propagates to higher values of  $k$ . When  $X(k, l, 0) = 0$  the  $p > 0$  coefficients are calculated by requiring the right-hand side of (20) to vanish, that is

$$2 \sum_{g=1}^{\infty} \frac{X(k, l, g)}{g(2l+g+1)} R(k, l, g, p) + D(k, l, p) = 0. \quad (27)$$

The  $C_{k-ll0}$  for  $k = 2l + 4n$  where  $n = 0, 1, 2, \dots$  are determined by the requirement of a normalisable wavefunction.

When condition (25) is applied and the 1-3 and 2-3 potentials are equal, the functions used in the general three-particle equations satisfy the relationships

$$R(k, l, g, p) = R'(k, l, g, p)$$

and

$$D(k, l, p) = D'(k, l, p).$$

In this limit the continuity equation (14) vanishes and the derivative continuity equations (15) and (16) become equal to (26). The equations for  $k = 2l + 2n + 2$  were (19) and (20). Equation (19) vanishes and (20) becomes equal to (26). The equations for  $k = 2l + 4n$ , (21) and (22), reduce to equation (27). Condition (25) places an extra restriction on the arbitrary coefficients of the general three-particle series. This completely specifies the arbitrary coefficients at  $k = 2l + 4n + 2$  but still leaves those with  $k = 2l + 4n$  undetermined.

Thus in the limiting case of the two identical finite mass particles the equations describing three non-identical particles reduce correctly to those for a symmetric eigenfunction of a Hamiltonian for two identical particles plus a third particle.

#### 4. The antisymmetric case

For an antisymmetric wavefunction

$$\Psi(r_1, r_2, \Omega) = \begin{cases} \exp(-\lambda_1 r_1 - \lambda_2 r_2) \sum_{ijlp} C_{ijlp} r_1^j r_2^l [e^{qr_1} \text{Ei}(-qr_1)]^p P_l(\Omega) / p! & r_1 > r_2 \\ -\exp(-\lambda_1 r_2 - \lambda_2 r_1) \sum_{ijlp} C_{ijlp} r_1^j r_2^l [e^{qr_2} \text{Ei}(-qr_2)]^p P_l(\Omega) / p! & r_1 < r_2 \end{cases} \quad (28)$$

which is identical to the general three-particle series (3) with

$$C_{ijlp} = -C'_{ijlp}. \quad (29)$$

The condition for an antisymmetric function  $\Psi(r_1, r_2, \Omega)$  to be continuous at  $r_1 = r_2 = r$  is

$$\Psi(r, r, \Omega) = 0.$$

For series (28) this implies

$$\sum_k C_{ijlp} = 0 \quad \text{for all } k, \quad (30)$$

which automatically guarantees derivative continuity.

Rewriting equation (30) as before gives

$$W(k, l, 0) C_{k-llp} = -2 \sum_{g=1}^{\infty} \frac{W(k, l, g)}{g(2l+g+1)} R(k, l, g, p).$$

The arbitrary coefficients arise when  $W(k, l, 0) = 0$ , that is when  $k = 2l + 4n + 2$ ;  $n = 0, 1, 2, \dots$ . The equations for three non-identical particles reduce to the equations for the antisymmetric function (28) in the limit of the 1-3 and 2-3 potentials being equal, assuming that condition (29) applies.

Applying (29) and (23) to  $C_{0000}$  yields

$$C_{0000} = C'_{0000} = 0.$$

Condition (29) determines the arbitrary coefficients of the general three-particle series with  $k = 2l + 4n$  completely. The arbitrary coefficients with  $k = 2l + 4n + 2$  are still undetermined. The first of these occurs at  $k = 2$ . Thus the antisymmetric series (28) starts at  $k = 2$  and propagates to higher values of  $k$ . This is in contrast with the series for the general three-particle system and the symmetric series which both start at  $k = 0$ .

#### 5. Conclusions

Once all non-arbitrary coefficients for the system of three distinguishable particles have been calculated, the special case with two of the particles identical may be obtained by making two of the interparticle potentials equal and requiring the wavefunction to be either symmetric or antisymmetric. Furthermore, the wavefunction describing a system of two non-interacting particles in the field of a third particle is simply obtained from the wavefunction for three non-identical interacting particles by setting the relevant potential term equal to zero.

This shows that up to the point of calculating the arbitrary coefficients, the case of two identical particles with either symmetric or antisymmetric functions and the

case of two non-interacting particles in the field of a third are given by the appropriate limit of the series for three non-identical interacting particles. That is, there is no need to specify the symmetry of the wavefunction, or the potentials, until the quantisation condition which results from the requirement of a normalisable wavefunction is applied. When calculating the arbitrary coefficients and the energy eigenvalues it is necessary to examine the asymptotic form of the wavefunction (Davis and Maslen 1983b), and it is only here that the form of the potentials and the symmetry are required.

It is interesting to note that the series for a symmetric function (24) starts at  $k=0$  whereas the series for an antisymmetric function (28) starts at  $k=2$ . In fact the wavefunctions to lowest order, when  $r_1 > r_2$  are

$$\Psi(r_1, r_2, \Omega) = \exp(-\lambda_1 r_1 - \lambda_2 r_2)$$

for a symmetric function and

$$\Psi(r_1, r_2, \Omega) = (r_1^2 - r_2^2) \exp(-\lambda_1 r_1 - \lambda_2 r_2)$$

for an antisymmetric function. This is clearly shown from the method of calculating the wavefunctions described in this paper, as the first arbitrary coefficient gives the lowest-order term in the series. This is less obvious in other methods. For example a helium-like atom in a  $^3S$ -state with no electron-electron interaction is described by an antisymmetric sum of a product of hydrogen wavefunctions. The hydrogen wavefunctions contain all non-negative integral powers of  $r$  but it is only after some algebraic manipulation that the  $r^0$  and  $r^1$  terms are seen to vanish in the helium  $^3S$  wavefunction.

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