Exact coupled set of ordinary differential equations for states of spherical symmetry of a three-body bound-state system*

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(Received 26 August 1974; revised manuscript received 4 June 1975)

The kinetic-energy operator derived by De Celles and Darling with center-of-mass motion separated is used to derive an orthonormal set of functions for the spherically symmetric states of a three-body bound-state system of arbitrary masses and charges. This approach allows the calculation of the energy E to be reduced to the solution of a coupled system of differential equations in one variable.

INTRODUCTION

The transformation of the kinetic-energy (KE) operator of an N-body quantum-mechanical system to a form which exhibits the separation of the internal and rotational motions and their coupling, the center-of-mass motion being separated out, has been made by various authors using different approaches,[1] and a derivation from a variational principle has been given in Ref. 1(c). Linden and Darling applied this method to the nuclear three-body problem and obtained a set of radial equations in terms of the three interparticle distances.[2] These radial equations are derived for a charge-independent general static exchange central interaction (combination of Wigner, Majorana, Bartlett, and Heisenberg forces), and a static nonexchange tensor interaction. In the derivation of these radial equations all symmetry properties, including the Pauli principle, were included.

Another application by Darling and collaborators,[3] in the case of three equal masses, is the ozone molecule where, however, different internal coordinates were employed. De Celles and Darling[4] derived a KE operator having the above-mentioned form for a system of three bodies with arbitrary masses, and their choice of internal variables is such that the purely internal part is a separable operator in these variables.

In this paper we shall find the characteristic solutions of the equations of this separable operator, and we shall use these orthonormal functions to transform the ground-state ($L=0$) bound-system problem to a set of coupled ordinary differential equations in the variable R. We also make a comparison with similar works.

KINETIC-ENERGY OPERATOR (KEO)

We give here briefly the main ideas of the approach used by Darling[1c] to derive the KEO. The point of departure is the correct Schrödinger equation for an N-particle system in Cartesian coordinates. The Cartesian coordinates are then partly expressed in terms of suitable generalized coordinates (corresponding to the $3N-6$ internal coordinates of the system), and partly expressed in terms of the infinitesimal operators of the continuous group of transformation (the group of parallel displacement, and the group of all spatial rotations). The advantage of this approach is that the Hamiltonian operator can be expressed in terms of the irreducible (numerical) matrices P_x, P_y, P_z, which are the representation of the components of the total orbital angular momentum under the three-dimensional rotation group. Separating out the translational motion, one gets the KE part of the Hamiltonian operator which is only a function of $3N-6$ internal variables and the P_x, P_y, P_z matrices. It must be emphasized that this KE part of the Hamiltonian operator is a Hermitian operator and consists of a purely vibrational part independent of the total angular momentum, a part depending quadratically on the angular momentum matrices, and another part depending linearly on these matrices and representing the interaction between the internal movement and the over-all rotation [for more details, see Ref. 1(c)].

In the case of the three-body problem, De Celles and Darling[4] determined a set of internal variables which made the purely internal operator a separable operator, and because of the Hermiticity, no first-order derivatives appear in this operator. With the body-fixed axes chosen as the principal axes of inertia, and the mentioned choice of internal variables, the KEO has the form ($\hbar=1$)

$$T=\frac{1}{2}\left(p_R^2+\frac{4}{R^2}\,p_\psi^2+\frac{1}{R^2\cos^2\psi}\,(2p_\lambda+\sin\psi P_z)^2 - \frac{1}{4R^2}-\frac{1}{R^2\sin^2\psi\cos^2\psi}\right) + \frac{1}{2}\left(\frac{P_x^2}{R^2(1-\cos\psi)/2}+\frac{P_y^2}{R^2(1+\cos\psi)/2}+\frac{P_z^2}{R^2}\right), \quad (1)$$

$$p_R = -i\frac{\partial}{\partial R},\quad p_\psi = -i\frac{\partial}{\partial \psi},\quad p_\lambda = -i\frac{\partial}{\partial \lambda}.$$

The square of one of these internal variables R is the moment of inertia about the axis perpendicular to the plane of the three particles through the center of mass, or since principal axes of inertia are employed, we have

$$R^2 = I_x + I_y .$$

In a plane with axes labeled $I_y^{1/2}$ and $I_x^{1/2}$, the variable R and the angle given by half of the second internal variable ψ play the role of polar coordinates, so that

$$I_y^{1/2} = R\cos(\psi/2),\quad I_x^{1/2} = R\sin(\psi/2). \tag{2}$$

The range of these variables is

$$0 < R < \infty,\quad 0 < \psi < \pi/2, \tag{3}$$

the latter being fixed by the fact that the principal axes have been chosen so that $I_x < I_y$. These variables determine the over-all size of the triangle formed by the three particles and the magnitudes of the moments of inertia. The third internal variable determines the skewness of the triangle formed by the three particles. It is also of the nature of an angle but its definition is somewhat more complicated. If one introduces a nonphysical three-dimensional space with axes 1, 2, 3, then the two vectors

$$\vec{x} = (x_1, x_2, x_3),\qquad \vec{y} = (y_1, y_2, y_3) \tag{4a}$$

and the vector

$$\vec{a} = (m_1^{1/2}, m_2^{1/2}, m_3^{1/2}) \tag{4b}$$

are mutually perpendicular,

$$\vec{a}\cdot\vec{x} = 0,\quad \vec{a}\cdot\vec{y} = 0,$$

because the origin is at the center of mass, and $\vec{x}\cdot\vec{y} = 0$ because the body-fixed axes are principal axes (the components of $\vec{x}$ and $\vec{y}$ are $m_k^{1/2}$ times the x_k and y_k components of the kth particle, i.e., the mass-reduced components). The third internal coordinate $\chi = \lambda/2$ $(-\pi \le \lambda \le \pi)$ is the angle shown on the Fig. 1, where the 3′ axis is along the vector $\vec{a}$ and the 1′ axis is perpendicular to the plane 3-0-3′.

There are no restrictions on the three masses of the interacting particles used in the derivation of Eq. (1). It is to be noted that the range of variation of the angle χ in Ref. 4 is only from 0 to π. Because of this, the element of integration is $\frac{1}{2}d\lambda\, d\psi\, dR$. But if one considers the reduced kinetic-energy operator[4,5] one can use directly the element of integration $d\lambda\, d\psi\, dR$. Also, we shall write in the following $T = T_v + T_p$, where T_v is the pure vibrational part of the K. E. operator.

S STATES

For the S states, the three angular momenta of rotation, P_x, P_y, P_z with respect to the three principal axes of inertia, are zero. The K. E. operator reduces to T_v. This operator is separable in the three variables R, ψ, λ, and the characteristic solutions can be expressed as a product of a radial part and an angular part. The angular part turns out to be a product of trigonometric functions with Jacobi polynomials. These form an orthonormal set of functions in terms of which an arbitrary function of ψ, λ can be expanded.

To solve the equation

$$T_v\Phi = E_c\Phi, \tag{5}$$

we write $\Phi = \Phi_1(R)\Phi_2(\lambda)\Phi_3(\psi)$ and proceed in the usual manner to obtain the separated differential equations

$$\frac{d^2\Phi_1}{dR^2} + \left(2E_c - \frac{s^2 - \frac{1}{4}}{R^2}\right)\Phi_1 = 0, \tag{6}$$

$$\frac{d^2\Phi_2}{d\lambda^2} + \nu^2\Phi_2 = 0, \tag{7}$$

$$\frac{d^2\Phi_3}{d\psi^2} + \left(\frac{s^2}{4} + \frac{1}{4\sin^2\psi\cos^2\psi} - \frac{\nu^2}{\cos^2\psi}\right)\Phi_3 = 0, \tag{8}$$

where s^2, ν^2 are separation constants. The function Φ_2 is cyclic in λ, with period 2π, as explained in Appendix B. This restricts ν to integer values.

CHARACTERISTIC FUNCTIONS AND EXPANSIONS

We consider first the differential equation (6). A solution which is continuous, finite, and satisfies this equation at all points including $R = 0$ and $R \to \infty$ is given in terms of the Bessel function $R^{1/2}J_s(R(2E_c)^{1/2})$. This solution is not square integrable over the range $(0, \infty)$, but we know that a square-integrable function $F_1(R)$, as is generally required by the physical conditions of quantum-mechanical problems, can be expanded in terms of $R^{1/2}J_s(R(2E_c)^{1/2})$ by the use of the well-known Fourier-Bessel expansion[6]

$$F_1(R) = \int_0^\infty R^{1/2}J_s(R(2E_c)^{1/2})(2E_c)^{1/2}\, d(2E_c)^{1/2} \times \int_0^\infty y^{1/2}J_s(y(2E_c)^{1/2})F_1(y)\, dy. \tag{9}$$

The expansion of a single-valued and periodic function of λ, $F_2(\lambda)$, in terms of the characteristic solution of the differential operator (7) is the well-known Fourier expansion

$$F_2(\lambda) = a_0 + \sum_{\nu=1}^{\infty} a_\nu\cos\nu\lambda + \sum_{\nu=1}^{\infty} b_\nu\sin\nu\lambda, \tag{10}$$

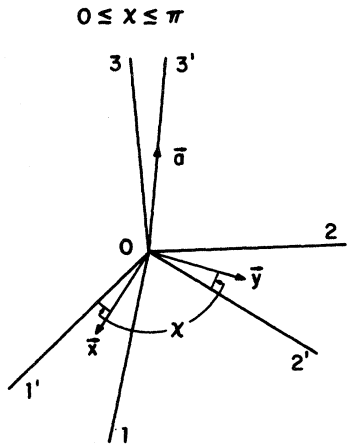

FIG. 1. Definition of the vectors $\vec{a}$, $\vec{x}$, and $\vec{y}$.

$$a_0=\frac{1}{2\pi}\int_0^{2\pi}F_2(\lambda)d\lambda,$$

$$a_\nu=\frac{1}{\pi}\int_0^{2\pi}F_2(\lambda)\cos\nu\lambda\,d\lambda, \tag{11}$$

$$b_\nu=\frac{1}{\pi}\int_0^{2\pi}F_2(\lambda)\sin\nu\lambda\,d\lambda.$$

The derivation of the characteristic solution of Eq. (8) will be treated in some detail, because it gives a relation between the Gauss hypergeometric differential equation and the Hill-type differential equation (8).[7] Titchmarsh[8] has treated the problem by reducing the Gauss hypergeometric equation to a form which eliminates the first-order differential operator, but we give in the following a simpler approach. The substitution $z=\cos^2\psi$ in Eq. (8) gives directly

$$\frac{d^2\Phi_3}{dz^2}+\frac{1}{2}\left(\frac{1}{z-1}+\frac{1}{z}\right)\frac{d\Phi_3}{dz}+\left(\frac{1-4\nu^2}{16}\frac{1}{z^2}+\frac{1}{16}\frac{1}{(z-1)^2}+\frac{4\nu^2-s^2-2}{16}\frac{1}{z(z-1)}\right)\Phi_3=0, \tag{12}$$

which has the Riemann P symbol

$$\Phi_3=P\begin{pmatrix}0 & 1 & \infty\\ \frac{1}{4}+\nu/2 & \frac{1}{4} & s/4 & z\\ \frac{1}{4}-\nu/2 & \frac{1}{4} & -s/4\end{pmatrix}. \tag{13}$$

The function Φ_3 can also be written in the form[9]

$$\Phi_3=z^{(1+2\nu)/4}(1-z)^{1/4}G, \tag{14}$$

where G is given by

$$G=P\begin{pmatrix}0 & 1 & \infty\\ 0 & 0 & \frac{1}{4}(s+2\nu+2) & z\\ -\nu & 0 & \frac{1}{4}(2\nu-s+2)\end{pmatrix}. \tag{15}$$

The solution of the Gauss hypergeometric differential equation

$$z(1-z)\frac{d^2G}{dz^2}+[c-(a+b+1)z]\frac{dG}{dz}-abG=0 \tag{16}$$

is of the form

$$G=P\begin{pmatrix}0 & 1 & \infty\\ 0 & 0 & a & z\\ 1-c & c-a-b & b\end{pmatrix}; \tag{17}$$

hence the differential equation (8) admits the solution

$$\Phi_3=z^{(1+2\nu)/4}(1-z)^{1/4}G(a,b,c,z), \tag{18}$$

where $G(a,b,c,z)$ is the Gauss hypergeometric function, and

$$a=\tfrac{1}{4}(s+2\nu+2),\quad b=\tfrac{1}{4}(2\nu-s+2),\quad c=1+\nu. \tag{19}$$

A second independent solution is given by

$$\Phi_3^s=z^{(1+2\nu)/4}(1-z)^{1/4}G(a,b,1,1-z) \tag{20}$$

The Wronskian of these solutions, as derived in Appendix A, is given by $W=2\Gamma(a+b)/\Gamma(a)\Gamma(b)$. The solution $G(a,b,c,z)$ is regular at $z=0$. At $z=1$,

$$G(a,b,c,z)\sim\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\ln\frac{1}{1-z}$$

so that the product $(1-z)^{1/4}G(a,b,c,z)$ tends to zero as $z\to 1$. Similar considerations apply to Φ_3^s. Hence Φ_3 and Φ_3^s are finite in the closed interval $(0,1)$. But the Gauss hypergeometric differential equation is not satisfied at $z=1$, when $a+b=c$, and the hypergeometric series diverges at this point. Since the physical conditions require that the differential equation be satisfied for all values of z including 0 and 1, we see that for this last condition to be satisfied, $G(a,b,c,z)$ must be a polynomial, i.e., a or $b=-n$, $n=0,1,2,3\ldots$. For these values of a or b, the Wronskian is null; i.e., the two solutions are linearly dependent,

$$G(a,b,1,1-z)=A_{n\nu}G(a,b,c,z),$$

where

$$A_{n\nu}=\frac{(-1)^n}{n!}\frac{\Gamma(1+n+\nu)}{\Gamma(1+\nu)}.$$

The function Φ_3 can be written as

$$\Phi_3 = z^{(1+2\nu)/4}(1-z)^{1/4}G(-n, 1+n+\nu; 1+\nu; z)\,. \qquad (21)$$

We now introduce in place of s the parameter κ as follows:

$$(s+2\nu+2)/4 = -\tfrac{1}{2}(\kappa/2-\nu) = -n, \quad s = -\kappa-2\,.$$

This has the advantage of simplifying the expression of the coupled-differential-equation system (32).

Since $n = 0, 1, 2, 3, \ldots$, this determines that $\kappa = 0, 2, 4, 6, \ldots$, and that $\nu = \kappa/2, \kappa/2-2, \kappa/2-4, \ldots, \nu \geq 0$. The solution (21) can be expressed in terms of the Jacobi polynomials through the relation

$$\frac{(\kappa/4-\nu/2)!}{(1+\nu)_{\kappa/4-\nu/2}} P^{\nu,0}_{(\kappa/2-\nu)/2}(1-2z) = G(-\tfrac{1}{2}(\kappa/2-\nu), 1+\nu/2+\kappa/4; 1+\nu; z)\,. \qquad (22)$$

We shall now keep this last notation and write the solution (21) as follows:

$$\Phi_3 \propto \rho^{(1+2\nu)/2}(1-\rho^2)^{1/4}P^{\nu,0}_{(\kappa/2-\nu)/2}(1-2\rho^2)\,, \qquad (23)$$

where we have substituted $z = \rho^2$.

The element of integration $d\psi$ is $dz/2z^{1/2}(1-z)^{1/2}$ for Eq. (21), and to change it to $\rho\,d\rho$ is equivalent of changing our orthogonal set of functions from (23) to $\rho^{\nu}P^{\nu,0}_{1/2(\kappa/2-\nu)}(1-2\rho^2)$. Our orthonormal set of functions will then be given by

$$v^{\nu}_{\kappa}(\lambda,\psi) = \left(\frac{\kappa+2}{\pi^3}\right)^{1/2} \cos\nu\lambda \times \rho^{\nu}P^{\nu,0}_{1/2(\kappa/2-\nu)}(1-2\rho^2) \times \begin{cases} 1, & \nu \neq 0 \\ \frac{1}{2}\sqrt{2}, & \nu = 0\,, \end{cases} \qquad (24)$$

$$w^{\nu}_{\kappa}(\lambda,\psi) = \left(\frac{\kappa+2}{\pi^3}\right)^{1/2} \sin\nu\lambda\; \rho^{\nu}P^{\nu,0}_{1/2(\kappa/2-\nu)}(1-2\rho^2)\,.$$

The element of integration is $\pi^2\rho\,d\rho\,d\lambda$, with $0<\rho<1$, $-\pi \leq \lambda \leq \pi$, $\rho = \cos\psi$.

We have written the functions (24) so that they be symmetric or antisymmetric with respect to the change $\lambda \to -\lambda$ ($\lambda \to 2\pi - \lambda$ if the range of λ is taken from 0 to 2π) (see Appendix B). We shall write in the following $u^{\nu}_{\kappa}(\lambda,\psi)$ to designate either $v^{\nu}_{\kappa}(\lambda,\psi)$ or $w^{\nu}_{\kappa}(\lambda,\psi)$.

The radial solution with Eqs. (24) are continuum wave functions for three free particles with total angular momentum zero. However, the internal motion of a system of particles can be such that there are relative internal angular momenta of one part of a system with respect to another part, as for example in a system containing internal rotators, even though these may counterbalance to yield a total angular momentum zero. There is just such a situation here for the three-particle system. This internal angular momentum is characterized by the functions which are somewhat analogous to the spherical harmonics $Y^m_l(\theta,\varphi)$ that characterize the angular momentum of a particle about the origin. Mathematically the correspondence is $\lambda \longleftrightarrow \varphi$, $\nu \longleftrightarrow m$ with the circular function in each case, $\psi \longleftrightarrow \theta$, $\kappa \longleftrightarrow l$; but the functional relation involves the Jacobi polynomials on the one hand, and the associated Legendre functions on the other. Physically the analogy is rather remote, for in the problem considered here both the functions of the λ and the ψ characterize only the different components in the internal vibrational motion in the plane of the particles where the internal angular momenta are thus always perpendicular to the plane of the three particles.

It turns out that Gronwall,[10] using a different approach for a fixed-nucleus system, succeeded in deriving an orthonormal set of functions which is equivalent to ours. Simonov,[11] in the case of three particles of the same mass, by quite a different but clever route has arrived for the S states at employing the same functional forms as the $u^{\nu}_{\kappa}(\lambda,\psi)$, and we have followed for simplicity his notation here. If one consults the entries under $L=0$ of his Table I, he shows the partition of the internal angular momentum in his coordinates.

Zickendraht[12] has also derived a KEO for the three-body system with arbitrary masses. After separating the center-of-mass motion the derivation he used consists in expressing a six-dimensional Laplacian operator in a particular set of hyperspherical coordinates. However, in our derivation the KEO is derived for an N-body system, as explained earlier, in a form depending only on the $3N-6$ internal variables, and the derivation of Eq. (1) is done by direct application to the case where $N=3$ (see Ref. 4). The internal part $O_s(L=0)$ of the KEO in Zickendraht's work is also separable, but is not Hermitian. Also our aim is different, for we are interested in solving a set of coupled ordinary differential equations [Eqs. (32)], as discussed later, whereas Zickendraht has constructed a variational function.

A slightly different approach for a fixed nucleus system has also been done by Laughlin and Amos.[13] We also mention the recent work of Whitten and Sims,[14] where a different approach is done to separate the internal motion from the rotational motion of the three-body problem.

TRANSFORMATION OF THE SOLUTION OF THE TOTAL HAMILTONIAN

We consider now the solution $\underline{\Psi}(R, \psi, \lambda)$ of the equation

$$(T+V)\underline{\Psi} = E\underline{\Psi}\,, \tag{25}$$

where $V(R, \psi, \lambda)$ is the total potential energy of interaction between three particles.[4] We write

$$\underline{\Psi}(R, \psi, \lambda) = \sum_{\kappa,\nu} \int_0^\infty (2E_c)^{1/2}\, d(2E_c)^{1/2}\, \underline{C}_{\kappa\nu}((2E_c)^{1/2}) \times R^{1/2} J_{-\kappa-2}(R(2E_c)^{1/2}) u_\kappa^\nu(\lambda, \psi)\,; \tag{26}$$

$\underline{\Psi}$ and $\underline{C}$ are column functions of dimension $2L+1$, L being the total orbital angular momentum. Substituting Eq. (26) in Eq. (25) gives

$$(T_v - E)\underline{\Psi} = \sum_{\kappa,\nu} \int_0^\infty (2E_c)^{1/2}\, d(2E_c)^{1/2} \{(E_c - E)\underline{C}_{\kappa\nu}((2E_c)^{1/2})\, R^{1/2} J_{-\kappa-2}(R(2E_c)^{1/2}) u_\kappa^\nu(\lambda, \psi)\} = -(T_p + V)\underline{\Psi}\,,$$

$$\underline{C}_{\kappa\nu}((2E_c)^{1/2})(E - E_c) = \int_{\lambda=0}^{2\pi} \int_0^{\pi/2} \int_0^\infty (T_p + V)\underline{\Psi} R^{1/2} J_{-\kappa-2}(R(2E_c)^{1/2}) u_\kappa^\nu(\lambda, \psi)\, d\lambda\, d\psi\, dR\,. \tag{27}$$

Substituting in this last equation for $\underline{\Psi}$ its expansion (26) gives the set of integral equations

$$\underline{C}_{\kappa\nu}((2E_c)^{1/2}) = \frac{1}{E - E_c} \sum_{\kappa'\nu'} \int_0^\infty \underline{C}_{\kappa'\nu'}((2E_c')^{1/2})\, K_{\kappa\nu}^{\kappa'\nu'}((2E_c)^{1/2}, (2E_c')^{1/2})(2E_c')^{1/2}\, d(2E_c')^{1/2}\,. \tag{28}$$

The symmetric kernel is given by

$$K_{\kappa\nu}^{\kappa'\nu'}((2E_c)^{1/2}, (2E_c')^{1/2}) = \int_0^{2\pi} \int_0^{\pi/2} \int_0^\infty R^{1/2} J_{-\kappa-2}(R(2E_c)^{1/2}) R^{1/2} J_{-\kappa'-2}(R(2E_c')^{1/2})\, u_\kappa^\nu(\lambda, \psi) u_{\kappa'}^{\nu'}(\lambda, \psi)\, dR\, d\lambda\, d\psi\,. \tag{29}$$

Recent work on the existence of the solution of a set of equations of the type (28) are given in Ref. 15.

An alternative approach to the problem is to express the solution of Eq. (25) in terms of the orthonormal set of angular functions $u_\kappa^\nu(\lambda, \psi)$. We write

$$\underline{\Psi} = \sum_{\kappa,\nu} \underline{F}_{\kappa\nu}(R) u_\kappa^\nu(\lambda, \psi)\,.$$

Written explicitly, this has the form

$$\begin{bmatrix} \Psi^L \\ \Psi^{L-1} \\ \vdots \\ \Psi^{-L} \end{bmatrix} = \sum_{\kappa,\nu} \begin{bmatrix} F_{\kappa\nu}^L \\ F_{\kappa\nu}^{L-1} \\ \vdots \\ F_{\kappa\nu}^{-L} \end{bmatrix} u_\kappa^\nu(\lambda, \psi)\,. \tag{30}$$

Since we have changed our element of integration from $dz/2z^{1/2}(1-z)^{1/2}$ to $\rho\, d\rho$, the wave function is correspondingly divided by a factor of $z^{1/4}(1-z)^{1/4}$. The operator of Eqs. (1) is now transformed to

$$\left(\frac{1}{f} T_v f\right)\Psi + \left(\frac{1}{f} T_p f\right)\Psi + V\Psi = E\Psi\,, \tag{31}$$

where $f = \sin^{1/2}\psi \cos^{1/2}\psi$.

We confine ourselves to states of spherical symmetry, for which

$$\left(\frac{1}{f} T_p f\right)\Psi = 0, \quad L = 0\,.$$

The wave function Ψ can now be written in the form

$$\Psi = \sum_{\kappa',\nu'} \chi_{\kappa'}^{\nu'}(R) u_{\kappa'}^{\nu'}(\lambda, \psi)\,,$$

and Eq. (31) reduces to

$$\sum_{\kappa',\nu'} u_{\kappa'}^{\nu'}(\lambda, \psi)\left(\frac{d^2}{dR^2} + 2E - \frac{(\kappa'+2) - \frac{1}{4}}{R^2}\right)\chi_{\kappa'}^{\nu'}(R) = 2V \sum_{\kappa',\nu'} u_{\kappa'}^{\nu'}(\lambda, \psi)\chi_{\kappa'}^{\nu'}(R)\,.$$

We multiply both sides by $u_\kappa^\nu(\lambda, \psi)$ and integrate with respect to λ, ψ to obtain

$$\left(\frac{d^2}{dR^2} + 2E - \frac{(\kappa+2)^2 - \frac{1}{4}}{R^2}\right)\chi_\kappa^\nu(R) = -\sum_{\kappa',\nu'} U_{\kappa\kappa'}^{\nu\nu'} \chi_{\kappa'}^{\nu'}(R)\,, \tag{32}$$

where

$$U_{\kappa\kappa'}^{\nu\nu'} = -2 \int_0^1 \int_0^{2\pi} u_\kappa^\nu(\lambda, \psi)\, V u_{\kappa'}^{\nu'}(\lambda, \psi) \pi^2 \rho\, d\rho\, d\lambda\,. \tag{33}$$

Equation (33) has to be divided by $\hbar^2$ if we do not take $\hbar = 1$. Similarly $2E$ in Eq. (32) would be replaced by $2E/\hbar^2$.

SOLUTION OF THE COUPLED SET OF DIFFERENTIAL EQUATIONS

We first note that if we take only the diagonal element of the interaction $U^{\nu\nu}_{KK}$ into consideration, Eq. (32) will take the form

$$\left(\frac{d^2}{dR^2} + 2E + U^{\nu\nu}_{KK}(R) - \frac{(\kappa+\frac{3}{2})(\kappa+\frac{5}{2})}{R^2}\right)\chi^{\nu}_{\kappa}(R) = 0 . \quad (34)$$

In the case of a Coulomb interaction, the potential function has been derived by De Celles and Darling.[4] It can be shown by simple inspection that the interaction potential $U^{\nu\nu}_{KK}(R)$ can be written as $C^{\nu\nu}_{KK}/R$, where $C^{\nu\nu}_{KK}$ is independent of R. Equation (34) reduces to the hydrogenlike form

$$\left(\frac{d^2}{dR^2} + 2E + \frac{C^{\nu\nu}_{KK}}{R} - \frac{(\kappa+\frac{3}{2})(\kappa+\frac{5}{2})}{R^2}\right)\chi^{\nu}_{\kappa}(R) = 0 . \quad (35)$$

The solution of this equation has been discussed by Titchmarsh, Ref. 8, p. 99. The solution has a discrete and a continuous spectrum. The discrete spectrum for the lowest-order radial function $\chi^0_0(R)$ is given by

$$2E_n = -\frac{(C^{00}_{00})^2}{4(\frac{3}{2}+n+1)^2}, \quad n = 0, 1, 2, 3 \ldots .$$

$C^{00}_{00} = 11.179\,454\,4$ a.u., which gives $E_0 = -2.499\,604$ a.u. for ^{4}He, compared to the experimental value of $-2.903\,72$ a.u. This represents 86% of the total energy, obtained with the zero-order wave function, a result comparable to that obtained with the zero-order wave functions of Laughlin and Amos.[13]

A more accurate calculation of the eigenvalue can be done by transforming either Eq. (32) or (34) into a set of coupled integral equations. This is the method adopted by Simonov[11] in case of Eq. (32). The derivation of the Green's function of Eq. (34) is discussed by Titchmarsh[8] for the case of a Coulomb interaction.

An alternative and interesting approach is to transform the set of differential equations (32) into a set of difference equations. Work along this line has already been done by Winter *et al.*,[16] where a two-dimensional difference equation was used. Because of the two dimensions, the number of pivotal points needed to obtain a result which would compete with the accuracy of the variational method is prohibitive, and the calculation of the energy was done by using numerical extrapolation. The reduction of the three-body problem to a coupled system of one-variable differential equations makes it likely that such a result could be achieved by using a difference scheme. Work along this line is actually in progress and will be reported later.

ACKNOWLEDGMENT

One of us (RMS) would like to thank Professor J. Van Kranendonk for his kind assistance and helpful discussions on various theoretical aspects of this work during the academic year he spent in the Department of Physics, University of Toronto.

APPENDIX A

For the differentiation of the function Φ_3 or Φ^s_3, we write

$$\Phi_3' = \frac{d\Phi_3}{d\psi} = \frac{d\Phi_3}{dz}\frac{dz}{d\psi} .$$

By direct differentiation we obtain ($c = \nu$)

$$\frac{d\Phi_3}{dz} = \frac{2c(1-z)-1}{4z(1-z)}\Phi_3 + z^{(2c-1)/4}(1-z)^{1/4}\frac{ab}{c}G(a+1, b+1, c+1; z),$$

$$\frac{dz}{d\psi} = -2\sin\psi\cos\psi = -2[z(1-z)]^{1/2}, \quad (A1)$$

$$\frac{d\Phi^s_3}{dz} = \frac{2c(1-z)-1}{4z(1-z)}\Phi^s_3 - z^{(2c-1)/4}(1-z)^{1/4}abG(a+1, b+1, 2, 1-z) .$$

Direct substitution of Eqs. (A1) in the expression of the Wronskian of Φ_3 and Φ^s_3 with respect to ψ gives

$$W = -2\left(\frac{2c(1-z)-1}{4}z^{c-1}G(a, b, c, z)G(a, b, 1, 1-z) - z^c(1-z)abG(a, b, c, z)G(a+1, b+1, 2, 1-z)\right.$$
$$\left. - \frac{2c(1-z)-1}{4}z^{c-1}G(a, b, 1, 1-z)G(a, b, c, z) - z^c(1-z)\frac{ab}{c}G(a, b, 1, 1-z)G(a+1, b+1, c+1, z)\right) . \quad (A2)$$

The expression (A2) is evaluated at $z = 1$. Since in our case $a + b = c$, the hypergeometric function $G(a, b, c, z)$ is divergent at this point. Use is thus made of the asymptotic expression of this function near $z = 1$. This is given by[17]

$$G(a, b, c, z) \sim \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\ln\frac{1}{1-z}, \quad (A3)$$

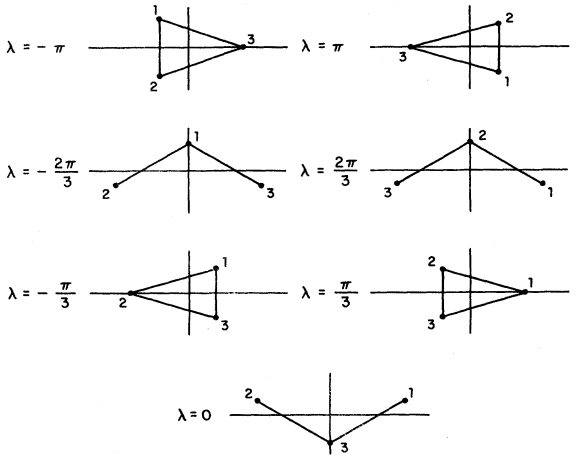

FIG. 2. Effect of the change of λ on the configuration of the triangle.

$$G(a+1,b+1,c+1,z)\sim\frac{\Gamma(c+1)\Gamma(a+1+b+1-c-1)}{\Gamma(a+1)\Gamma(b+1)}\times\frac{1}{(1-z)^{a+1+b+1-c-1}}\sim\frac{\Gamma(c+1)}{\Gamma(a+1)\Gamma(b+1)}\frac{1}{1-z}\,. \tag{A4}$$

Noting that

$$\lim_{z\to 1}(1-z)\ln(1-z)\to 0\,,$$

we see that the only contribution is obtained from the last term in the expression (A2). The first and the third terms cancel. Hence

$$W=2\frac{ab}{c}\frac{\Gamma(c+1)}{\Gamma(a+1)\Gamma(b+1)}=2\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}\,. \tag{A5}$$

APPENDIX B

From Fig. 1, it is clear that a change $\lambda\to\lambda+2\pi$ results in a change of the sign of the $\vec{x}$ and $\vec{y}$ in the primed system of coordinates defined by De Celles and Darling[4]. This results in an inversion through the origin in the plane of the three particles, which is equivalent to a rotation by π around the Z axis.

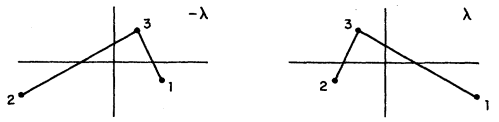

FIG. 3. Effect of the change $\lambda\to-\lambda$ on the configuration of the triangle.

Consequently a change $\lambda\to\lambda+2\pi$ followed by a rotation by π about the z axis results in an identical configuration. $\underline{\Psi}(\lambda+2\pi)=e^{i\pi P_z}\underline{\Psi}(\lambda)$; $\underline{\Psi}(\lambda)$ is periodic if K is even, antiperiodic if K is odd, where K is the component of the orbital angular momentum along the Z axis perpendicular to the plane of the three particles.[18] For spherically symmetric states, $\Psi(\lambda+2\pi)=\Psi(\lambda)$. This restricts ν to integer values as mentioned for Eq. (7).

The effect of the change of λ on the configuration of the triangle can be easily deduced as shown in Fig. 2, using Eqs. (B1),[4]

$$\begin{aligned} r_{12}^2&=(R^2/2m_{12})[1+\cos\psi\cos\lambda]\,,\\ r_{23}^2&=(R^2/2m_{23})[1+\cos\psi\cos(\lambda+2\delta_1)]\,,\\ r_{13}^2&=(R^2/2m_{13})[1+\cos\psi\cos(\lambda-2\delta_2)]\,, \end{aligned} \tag{B1}$$

and the results of Appendix B of Ref. 4. Figure 2, for simplicity, is for the case of three equal masses, for which $\delta_1=\delta_2=\pi/3$.

We finally consider the interchange of two identical particles 1 and 2 and the application of the Pauli exclusion principle. The substitution $\lambda\to-\lambda$ changes the twisted configuration of the triangle at λ to that at $-\lambda$ as shown in Fig. 3. The spatial wave function must be symmetric or antisymmetric under the following operations which interchange the identical particles 1, 2: $\lambda\to-\lambda$, and rotation by π around the y axis. Since for the ground state the wave function is spherically symmetric, this implies that the spatial wave function [Eqs. (24)] must be either symmetric (singlet state) or antisymmetric (triplet state) with respect to the change $\lambda\to-\lambda$.

*This work has been supported by a grant from the National Research Council of Canada.

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