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A Kontorovich–Lebedev representation for zero-range potential eigensolutions

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Abstract

A novel mathematically simple Kontorovich–Lebedev representation of solutions to the Schrödinger equation for a three-particle problem where two of them interact via a zero-range potential is developed. The asymptotic limits and regularity properties are studied. The connection between the representations for $E > 0$ and $E < 0$ is also discussed.

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1. Introduction

Since the beginning of quantum mechanics, the three-body problem has been of fundamental importance in atomic physics. This had motivated researchers to develop a variety of mathematical techniques to find approximate and exact solutions. Even with all the efforts of the community of theorists, only a few simple cases have been solved exactly in closed form [1]. These solvable models have motivated approximate methods for general systems [2]. Conversely, it is valuable to find models whose exact solution employs techniques that relate closely to approximate methods for general physical systems. In this paper we solve a model using methods developed for the states of three charged particles [3].

Since its first application in 1936 by Fermi to the study of neutron scattering, the use of zero-range potentials (ZRPs) has been applied to different areas of physics (see [1] and references therein). One of the reasons for their wide application is that in spite of their simplicity they very often retain essential physical features of real systems. ZRPs can be understood as a simplification of a more general technique since it can be shown that for low energy and in a limited energy region, the Schrödinger equation for two-body problems involving short-range potentials is equivalent to a free-particle Schrödinger equation with the following boundary condition:

$$\left.\frac{\partial(r\psi)}{\partial r}\right|_{r\to r_0} = M(E) \tag{1}$$

where $M(E)$ is an analytic function of the energy E and r_0 is any point of the space under consideration.

The interaction of equation (1) is exact for two-body problems [4], but it is not readily adapted to three-body problems [5]. To apply this interaction to three-body problems one can introduce the ZRP defined by taking the limit $r_0 \to 0$, leading to the condition

$$\frac{1}{r\psi}\frac{\partial(r\psi)}{\partial r}\bigg|_{r\to 0} = -1/a \tag{2}$$

where a is the scattering length. A free-particle Schrödinger equation with equation (2) as a boundary condition is equivalent to a Schrödinger equation with a short-range potential given by the ZRP. The simplest case is the one-dimensional potential where the ZRP is given by a delta function. In three dimensions, the potential $V(\boldsymbol{r})$ differs from the delta function by including an additional term [1]

$$V(\boldsymbol{r}) = \frac{2\pi}{a}\delta(\boldsymbol{r})(1 + \boldsymbol{r}\cdot\nabla_{\boldsymbol{r}}). \tag{3}$$

The equivalence between the boundary conditions and ZRPs applies to systems where only the S wave is relevant [5], i.e., at very low energies and in a limited energy region. This is the situation observed in the Bose–Einstein condensates where one of the more relevant parameters involved is the scattering length. Nielsen and Macek [6] have shown that the recombination process in a Bose–Einstein condensation can be modelled by a ZRP. This is our main interest. In this paper we consider the first step to find the closed-form solution for the systems where three particles interact via ZRPs.

The equivalence discussed in the previous paragraph leads to problems where the Schrödinger equation (in a three- or n-body problem) is separable but the boundary conditions are not. There are different methods that can be used in that sort of problem, but most of them lead to integral equations [7]. In this paper we use a method which is closely related the one used by Macek and Ovchinnikov [3] to study the three-body Coulomb potential. In this paper we will solve the three-body problem where two of the particles interact via ZRP using a notation that emphasizes the connection with the earlier work [3].

The Schrödinger equation for ZRPs is just the free-particle equation and is therefore separable in many coordinate systems. Following [3] we choose hyperspherical coordinates. One coordinate R, the hyper-radius, has dimensions of length and the other five are dimensionless angles, denoted collectively by $\hat{\boldsymbol{R}}$ [8]. The solution of the free-particle Schrödinger equation in these coordinates is given by a linear superposition of the separable solutions. The most general solution is

$$\Psi = \int_c A(\nu)S(\nu,\hat{\boldsymbol{R}})R^{1/2}Z_\nu(KR)\,\mathrm{d}^2\nu \tag{4}$$

where ν is a separation constant, Z_ν is a Bessel function and $S(\nu,\hat{\boldsymbol{R}})$ is a solution of the angular part of the free-particle Schrödinger equation. In order to satisfy the boundary conditions on ψ the function $S(\nu,\hat{\boldsymbol{R}})$ must be irregular at $\alpha = 0$ and regular at $\alpha = \pi/2$. The coefficients $A(\nu)$ and the contour are chosen so that Ψ satisfies the non-separable boundary conditions of equation (2). The non-separable boundary conditions then give equations for $A(\nu)$ and conditions that fix the contour of integration.

To connect this standard problem (4) with the method of [3] we note that these authors defined a set of Sturmian angle eigenfunctions by replacing the hyper-radius by an eigenvalue $\rho_j(\nu)$ in the Schrödinger equation. Thus they set

$$\left[\Lambda^2 + \rho_j(\nu)2C(\hat{\boldsymbol{R}})\right]S_j(\nu,\hat{\boldsymbol{R}}) = (\nu^2 - 1/4)S_j(\nu,\hat{\boldsymbol{R}}) \tag{5}$$

where Λ^2 is the generalized angular momentum operator, ν is a parameter, $\rho_j(\nu)$ is the Sturmian eigenvalue and $S_j(\nu, \hat{\boldsymbol{R}})$ the angle Sturmian eigenfunction. These Sturmian functions are then employed in a Kontorovich–Lebedev-like transform [9–13]. The main idea is to expand the angular part of the solution in terms of the Sturmians and use it as the kernel in the Kontorovich–Lebedev transform

$$\Psi(R, \hat{\boldsymbol{R}}) = \sum_n \int_c A_n(\nu) S_n(\nu, \hat{\boldsymbol{R}}) R^{1/2} Z_\nu(K R) \nu \, \mathrm{d}\nu. \tag{6}$$

The substitution of $\Psi(R, \hat{\boldsymbol{R}})$ from equation (6) into the Schrödinger equation leads to a set of coupled difference equations for the coefficients $A_n(\nu)$ which can be solved by using a variety of methods.

In the present case we define a function $\rho(\nu)$ by replacing R by $\rho(\nu)$ in the boundary conditions of equation (2), rather than in the Schrödinger equation. The boundary conditions on the complete function Ψ of equation (4) then give a three-term recurrence relation for the coefficients $A(\nu)$, just as for the Coulomb problem. Because we define the eigenvalue $\rho(\nu)$ by the boundary conditions, our angle functions $S(\nu, \hat{\boldsymbol{R}})$ are not Sturmian eigenfunctions. We show in section 2 that these functions have many, but not all, of the properties of Sturmian functions, therefore, we refer to them as psuedo-Sturmian functions. The main body of this paper discusses the contour of integration and its relation to the boundary conditions of the complete wavefunction.

The KL integral representation has two disadvantages from the physical point of view [9–12]. One is that it is often not possible to interchange limits from outside to inside the integral. For example, in the case of (6) it is possible to take the limit $R \to \infty$ inside the integral only if the integral converges after taking the limits of the Bessel function. This imposes stronger conditions on the coefficients $A_n(\nu)$ than does the requirement that the integral converge before taking the limits. As a consequence, it is difficult to match boundary conditions at large R.

New techniques must be devised to do this. One of the purposes of this paper is to devise methods to match boundary conditions at large R. We do this by finding a new integral representation of functions that are known in conventional Jacobi coordinates.

The second disadvantage is that the coefficient $A(\nu)$ in the KL representation often has poles which complicate numerical integration over the separation constant. In this paper we will write the solution of a zero-range potential problem as a KL-like representation that is free of poles. In section 2 we will present the problem and its closed-form solution. In section 3 we introduce the KL-like integral representation and study its limiting properties. In section 4 we close with some concluding remarks.

2. Hyperspherical pseudo-Sturmian functions

Hyperangle–Sturmian functions are defined for Coulomb potentials by equation (5). In this section we will define pseudo-Sturmian functions for ZRPs. Actually, such functions were implicitly introduced by Nielsen and Macek [6] in their discussion of three-body recombination. A related set of Sturmians has been discussed by Khrebtukov and Macek [14] and Macek *et al* [15]. These functions have many, but not all, of the properties of Sturmians, hence they are referred to as psuedo-Sturmians.

2.1. Pseudo-Sturmian functions for ZRPs

The angular eigenvalue equation for the case of three particles where only two of them interact via ZRPs is given by

$$[\Lambda^2 - (\nu^2 - 4)]S(\nu, \hat{\boldsymbol{R}}) = 0 \tag{7}$$

where

$$\Lambda^2 = -\frac{1}{\sin^2\alpha\cos^2\alpha}\frac{\partial}{\partial\alpha}\left(\sin^2\alpha\,\cos^2\alpha\frac{\partial}{\partial\alpha}\right) + \frac{L_{r_1}^2}{\sin^2\alpha} + \frac{L_{r_2}^2}{\cos^2\alpha}. \tag{8}$$

The equations are written in terms of the mass-scaled Jacobi coordinates r_1 and r_2. The hyperspherical coordinates are given by the hyper-radius $R = \sqrt{r_1^2 + r_2^2}$, the hyperangle $\alpha = \arctan(r_1/r_2)$ and the direction vectors $\hat{\boldsymbol{r}}_1$ and $\hat{\boldsymbol{r}}_2$.

The pseudo-Sturmian function $S(\nu, \hat{\boldsymbol{R}})$ must also satisfy the boundary condition

$$\left[\frac{\partial(\sin\alpha S)}{\partial\sin\alpha} + \rho(\nu)(\sin\alpha\, S)\right]_{\alpha\to 0} = 0. \tag{9}$$

As we can see, the eigenvalue $\rho(\nu)$ appears in the boundary condition. This sort of relation defines a pseudo-Sturmian boundary condition instead of a Sturmian one, because it depends on the eigenvalue of equation (7).

Due to the short range of the potential, the total angular momentum of the system is chosen equal to zero. Higher angular momenta could be considered, but are expected to be less important than $L = 0$ in regions where the ZRP models are used. The angular momenta $L_{r_1}^2$ and $L_{r_2}^2$ are then set equal to zero, $L_{r_1}^2 = L_{r_2}^2 = 0$.

To completely fix the solutions of equation (7) an additional boundary condition is needed. This additional boundary condition is taken at $\alpha = \pi/2$. The eigensolution of equation (7) regular at $\alpha = \pi/2$ is

$$S^{(1)}(\nu, \alpha) = \frac{\sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right]}{\sin\alpha\,\cos\alpha}. \tag{10}$$

The boundary condition (9) gives the expression

$$\rho^{(1)}(\nu) = a\nu\frac{\cos\left(\frac{\pi}{2}\nu\right)}{\sin\left(\frac{\pi}{2}\nu\right)} \tag{11}$$

for the eigenvalue $\rho(\nu)$.

A second solution of equation (7) is

$$S^{(2)}(\nu, \alpha) = \frac{\cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right]}{\sin\alpha\cos\alpha}. \tag{12}$$

This function is not regular at $\alpha = \pi/2$, instead one has

$$\frac{\partial}{\partial\alpha}\left(\cos\alpha\, S^{(2)}(\nu, \alpha)\right)\Big|_{\alpha=\frac{\pi}{2}} = 0. \tag{13}$$

Equation (9) leads to the following form for the eigenvalue $\rho(\nu)$:

$$\rho^{(2)}(\nu) = -a\nu\frac{\sin\left(\frac{\pi}{2}\nu\right)}{\cos\left(\frac{\pi}{2}\nu\right)}. \tag{14}$$

The boundary conditions at $\alpha = \pi/2$ are Sturmian boundary conditions because they are independent of the eigenvalue $\rho(\nu)$. The eigenfunctions given by equations (10) and (12) are linearly independent solutions of equation (7). Both of them satisfy Sturmian boundary conditions at $\alpha = \pi/2$ and pseudo-Sturmian conditions at $\alpha = 0$. Thus the functions $S^{(1,2)}$ are not Sturmian functions; and for that reason we call them pseudo-Sturmian functions. As we shall see they lead to solutions with different asymptotic behaviour at large R.

3. Three-term recurrence relations

In this section we apply the method described in section 1 to the wavefunctions for three particles where two of them interact via ZRPs.

The time-independent Schrödinger equation for three particles in mass-scaled coordinates is

$$\left[-\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2\right]\Psi = E\Psi. \tag{15}$$

The ZRP is included via the boundary condition where the logarithmic derivative of the function $r_1\Psi$ is fixed by

$$\left[\frac{\partial(r_1\Psi)}{\partial r_1} + \frac{1}{a}(r_1\Psi)\right]_{r_1\to 0} = 0. \tag{16}$$

In hyperspherical coordinates $r_1 = R\sin\alpha$, $r_2 = R\cos\alpha$ the Schrödinger equation (15) is

$$\left[\frac{1}{R^5}\frac{\partial}{\partial R}\left(R^5\frac{\partial}{\partial R}\right) + \frac{\Lambda^2}{R^2} + K^2\right]\Psi = 0 \tag{17}$$

where $K^2 = 2E$, the operator Λ^2 is defined by (8), and the boundary condition (16) is

$$\left[\frac{\partial(\sin\alpha\,\cos\alpha\Psi)}{\partial\alpha} + \frac{R}{a}(\sin\alpha\,\cos\alpha\Psi)\right]_{\alpha\to 0} = 0 \tag{18}$$

which is clearly non-separable in hyperspherical coordinates. In the last equation we introduced $\cos\alpha$ to simplify subsequent analysis. These changes do not modify the boundary conditions on Ψ.

Equations (17) and (18) represent a mathematical problem where the differential equation is separable in hyperspherical coordinates but the boundary conditions are not. Only one Sturmian is necessary to describe the dynamics of the problem and we have the general solution

$$\Psi(\alpha, R) = \frac{1}{R^2}\int_c A(\nu)S(\nu,\alpha)Z_\nu(KR)\,\mathrm{d}\nu^2. \tag{19}$$

This solution is a superposition of separable solutions with a sum over the separation constant chosen to satisfy the boundary condition (18).

The pseudo-Sturmian function $S(\nu,\alpha)$ was studied in the last section. The Bessel function $Z_\nu(KR)$ is the solution of equation (17) with the operator Λ^2 replaced by its eigenvalue. In this respect we have different choices, i.e., we can use the functions $H_\nu^{(1)}(KR)$, $H_\nu^{(2)}(KR)$ and $J_\nu(KR)$ which lead to solutions with outgoing [16], incoming and outgoing–incoming asymptotic behaviour when $E > 0$ and $K^2 = k^2 - 1/a^2$; for $E < 0$ we use $K_\nu(\mathcal{K}R)$ [16], with $\mathcal{K}^2 = 1/a^2 - k^2$.

The function $S(\nu,\alpha)Z_\nu(KR)$ satisfies the Schrödinger equation and we choose the separation constant $A(\nu)$ and the contour c to satisfy the boundary condition

$$\int_c\left[\frac{1}{R}\frac{\partial(\sin\alpha\,\cos\alpha\Psi)}{\partial\alpha} + \frac{1}{a_i}(\sin\alpha\,\cos\alpha\Psi)\right]_{\alpha\to 0}\mathrm{d}\nu^2 = 0. \tag{20}$$

The identity

$$\frac{2\nu}{KR}Z_\nu(KR) = Z_{\nu+1}(KR) + Z_{\nu-1}(KR) \tag{21}$$

allows us to rewrite equation (20) as follows:

$$\int_c A(\nu)\frac{\partial(\sin\alpha\ \cos\alpha S(\nu,\alpha))}{\partial\alpha}Z_{\nu+1}(KR)\,\mathrm{d}\nu+\int_c A(\nu)\frac{\partial(\sin\alpha\ \cos\alpha S(\nu,\alpha))}{\partial\alpha}Z_{\nu-1}(KR)\,\mathrm{d}\nu + \int_c A(\nu)\frac{2\nu}{aK}(\sin\alpha\ \cos\alpha\ S(\nu,\alpha))Z_\nu(KR)\,\mathrm{d}\nu=0. \tag{22}$$

At this point we introduce a restriction on the contour c and the coefficient $A(\nu)$. In equation (22) the Bessel functions are evaluated at different values of the indices ν and $\nu\pm1$. To obtain three integrals evaluated at the same value of ν we close each of the contours c to connect the functions $Z_{\nu\pm1}$ with Z_ν. This is possible because the contribution at infinity can be neglected and we require that the function $A(\nu)$ does not have poles inside the contour connecting ν and $\nu\pm1$. With this constraint we can rewrite the last equation as

$$\int_c\left[A(\nu-1)\frac{\partial(\sin\alpha S(\nu-1,\alpha))}{\partial\sin\alpha}+A(\nu+1)\frac{\partial(\sin\alpha S(\nu+1,\alpha))}{\partial\sin\alpha} + A(\nu)\frac{2\nu}{aK}(\sin\alpha S(\nu,\alpha))\right]Z_\nu(KR)\,\mathrm{d}\nu=0. \tag{23}$$

If the integrand in equation (23) vanishes, then the integral will also. This condition combined with equation (9) gives a recurrence relation for the coefficient $A(\nu)$

$$\left[A(\nu-1)\rho(\nu-1)S(\nu-1,\alpha)+A(\nu+1)\rho(\nu+1)S(\nu+1,\alpha)+A(\nu)\frac{2\nu}{K}S(\nu,\alpha)\right]_{\alpha\to0}=0. \tag{24}$$

The use of the expressions for $S(\nu,\alpha)$ and $\rho(\nu)$ from equations (10) and (11) of the previous section gives a three-term recurrence relation (TTRR)

$$\sin\left(\frac{\nu-1}{2}\pi\right)\rho(\nu-1)A(\nu-1)+\sin\left(\frac{\nu+1}{2}\pi\right)\rho(\nu+1)A(\nu+1) + \frac{2\nu}{K}\sin\left(\frac{\nu}{2}\pi\right)A(\nu)=0 \tag{25}$$

for the regular Sturmian and

$$\cos\left(\frac{\nu-1}{2}\pi\right)\rho(\nu-1)A(\nu-1)+\cos\left(\frac{\nu+1}{2}\pi\right)\rho(\nu+1)A(\nu+1) + \frac{2\nu}{K}\cos\left(\frac{\nu}{2}\pi\right)A(\nu)=0 \tag{26}$$

for the irregular Sturmian.

These TTRRs can be easily solved in exact form. To see this, substitute (11) for $\rho(\nu)$ and the relation $\cos\left[(\nu\pm1)\frac{\pi}{2}\right]=\mp\sin\left[\nu\frac{\pi}{2}\right]$ so that equations (25) and (26) together with the definition $B(\nu)=\nu A(\nu)$ give

$$B(\nu-1)-B(\nu+1)=\frac{2}{Ka}B(\nu). \tag{27}$$

By direct substitution one can verify that the general solution of (27) is

$$B(\nu)=\left[A_1\,\mathrm{e}^{-\nu\alpha_k}+A_2\,\mathrm{e}^{(\alpha_k\pm\mathrm{i}\pi)\nu}\right]F(\nu) \tag{28}$$

where α_k is defined by the relation $\sinh\alpha_k=1/Ka$, $A_{1,2}$ are constants to be determined and $F(\nu)$ is an arbitrary function with unit period, i.e., $F(\nu+1)=F(\nu)$.

With the results obtained for $A(\nu)$ and the definition of the pseudo-Sturmian functions (10) and (12) we have two formal solutions, apart from an overall constant; namely

$$\Psi^{(a)}(\alpha, R) = \frac{1}{R^2 \sin\alpha \, \cos\alpha} \int_c \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] Z_\nu(KR)\,\mathrm{d}\nu \tag{29}$$

and

$$\Psi^{(b)}(\alpha, R) = \frac{1}{R^2 \sin\alpha \, \cos\alpha} \int_c \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] Z_\nu(KR)\,\mathrm{d}\nu \tag{30}$$

where we assume $F(\nu) = 1$ and take $A_2 = 0$.

Until the boundary is selected and the convergence of the integral has been verified, these are only formal solutions of the Schrödinger equation. In the following sections we will find appropriate Bessel functions and contours so that the integrals converge and the solutions have the desired form in the asymptotic regions.

4. Wavefunctions

When only two of the three particles interact via ZRPs it is possible to solve the Schrödinger equation (16) satisfying the boundary condition (18) in, e.g., Cartesian coordinates. In the general case where all the particles interact, the problem becomes much more difficult since the boundary conditions do not separate in any coordinate system. It seems possible to solve the general case using the method of the previous section, but satisfying boundary conditions at large R is difficult. It is then useful to employ the method in the simplest case, since this will test techniques for matching boundary conditions at large R.

The solutions of equation (16) satisfying the boundary condition (18) in Cartesian and hyperspherical coordinates are

$$\Psi^{(1)}(\alpha, R) = \frac{\mathrm{e}^{-r_1/a}}{r_1}\frac{\sin(kr_2)}{r_2} = \frac{\mathrm{e}^{-R\sin\alpha/a}}{R\sin\alpha}\frac{\sin(kR\cos\alpha)}{R\cos\alpha} \tag{31}$$

and

$$\Psi^{(2)}(\alpha, R) = \frac{\mathrm{e}^{-r_1/a}}{r_1}\frac{\cos(kr_2)}{r_2} = \frac{\mathrm{e}^{-R\sin\alpha/a}}{R\sin\alpha}\frac{\cos(kR\cos\alpha)}{R\cos\alpha}. \tag{32}$$

The energy of the system $E = k^2/2 - 1/2a^2$ can be greater or less than zero depending upon whether k is greater or less than $1/a$. The first solution $\Psi^{(1)}(\alpha, R)$ of equation (31) is regular at $\alpha = \pi/2$ ($R \neq 0$) while the second, $\Psi^{(2)}(\alpha, R)$ of equation (31), is irregular at that point.

In this section we will study different Kontorovich–Lebedev representations of these solutions. We find apparently different expressions as E is greater or less than zero. We start with $E < 0$ since one can use the KL transform and standard integrals in this case.

4.1. $E < 0$

To obtain a Kontorovich–Lebedev integral representation for $\Psi^{(1,2)}(\alpha, R)$ we use the equation [10]

$$\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \cosh(\beta x) K_x(\rho)\,\mathrm{d}x = \frac{\pi}{2}\mathrm{e}^{-\rho\cosh\beta} \tag{33}$$

where $\rho > 0$ and $|\mathrm{Im}\,\beta| < \pi/2$. The restrictions are fulfilled for the functions considered here since we use the following expressions for β and ρ in equation (33):

$$\beta_k = \alpha_k \pm \mathrm{i}\left(\tfrac{\pi}{2} - \alpha\right) \qquad \rho = \mathcal{K}R. \tag{34}$$

Using the addition properties of the hyperbolic functions to rewrite $\cosh(x)$ on both sides of equation (33) we get

$$\frac{1}{\mathrm{i}\pi}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\cosh(\alpha_k\nu)\cos\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}\nu = \mathrm{e}^{-\mathcal{K}R\cosh(\alpha_k)\sin(\alpha)}\cos[\mathcal{K}R\sinh(\alpha_k)\cos(\alpha)] \tag{35}$$

and

$$\frac{1}{\mathrm{i}\pi}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\sinh(\alpha_k\nu)\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}\nu = \mathrm{e}^{-\mathcal{K}R\cosh(\alpha_k)\sin(\alpha)}\sin[\mathcal{K}R\sinh(\alpha_k)\cos(\alpha)]. \tag{36}$$

The integrals on the left-hand side of equations (35) and (36) are Kontorovich–Lebedev representations for the functions on the right-hand side. They can be directly compared with the definitions given by Lebedev [9–11].

Taking into account the symmetry properties of the hyperbolic and Bessel functions with respect to the integration variable ν and after some algebra we obtain expressions for equations (35) and (36) where the integrand is the product of a solution of the TTRR given by equation (28), regular and irregular pseudo-Sturmians and the Bessel function $K_\nu(\mathcal{K}R)$. To write a Kontorovich–Lebedev representation of the functions $\Psi^{(1)}$ and $\Psi^{(2)}$ we only need to introduce the definitions

$$\cosh(\alpha_k) = \frac{1}{\mathcal{K}a} \rightarrow \sinh(\alpha_k) = \frac{k}{\mathcal{K}} \tag{37}$$

where k is defined by $k^2 = 1/a^2 - K^2$ and $E < 0$. Then we have

$$\Psi^{(1)}(\alpha, R) = \frac{1}{\mathrm{i}\pi}\frac{1}{R^2\sin\alpha\cos\alpha}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\mathrm{e}^{-\alpha_k\nu}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}u \tag{38}$$

and

$$\Psi^{(2)}(\alpha, R) = \frac{1}{\mathrm{i}\pi}\frac{1}{R^2\sin\alpha\cos\alpha}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty}\mathrm{e}^{-\alpha_k\nu}\cos\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}u. \tag{39}$$

In this way we have obtained a KL representation for $E < 0$. These are given by $\Psi^{(a,b)}(\alpha, R)$ of equations (29) and (30) where the contour c goes from $\nu = -\mathrm{i}\infty$ to $\nu = \mathrm{i}\infty$ and the normalization constants are equal to $1/\mathrm{i}\pi$.

Our main concern is the representation for $E > 0$. Here we will see that a generalization of the KL transform is needed to transform the solutions in Jacobi coordinates to hyperspherical coordinates.

4.2. $E > 0$

Based on the formal solution (29) and using the Bessel functions for $E > 0$ we write

$$\tilde{\Psi}^{(1)}(\alpha, R) = \frac{1}{R^2\sin\alpha\,\cos\alpha}\left[\int_{C_1}\mathrm{e}^{-\nu\alpha_k}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]H_\nu^{(2)}(KR)\,\mathrm{d}\nu + \int_{C_2}\mathrm{e}^{-\nu\alpha_k}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]H_\nu^{(1)}(KR)\,\mathrm{d}\nu\right]. \tag{40}$$

The function $\tilde{\Psi}^{(1)}(\alpha, R)$ is a linear combination of two contour integrals. We choose C_1 to start at $\mathrm{i}\infty$ going along the imaginary axis towards the origin at $\nu = 0$, then turning around to the positive side of the real ν-axis and going to a large real value $\nu = \nu_N$. The contour C_2 starts at $-\mathrm{i}\infty$ and goes along the imaginary axis towards the origin at $\nu = 0$, then turns around

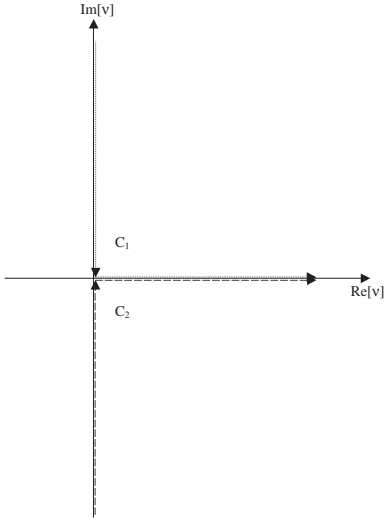

Figure 1. Contours C_1 and C_2 used to define the function $\tilde{\Psi}^{(1,2)}(\alpha, R)$ in equations (40) and (53).

to the positive side of the real ν-axis and goes to the point $\nu = \nu_N$. The two contours are shown in figure 1. The wavefunction $\tilde{\Psi}^{(1)}(\alpha, R)$ should be understood as the function which results after taking the limit $\nu_N \to \infty$ in both integrals simultaneously. The limit procedure defines $\tilde{\Psi}^{(1)}(\alpha, R)$ as the sum of two well-defined functions. It is necessary to sum both terms because each of the integrals separately diverges in the limit of $\nu_N \to \infty$. But if one takes the sum first and then the limit, the function is well defined. A completely similar analysis can be done using the second solution of the TTRR relation and/or the irregular pseudo-Sturmian function.

The procedure discussed above gives the following form for $\Psi^{(1)}(\alpha, R)$:

$$\begin{aligned}\tilde{\Psi}^{(1)}(\alpha, R) = \frac{1}{R^2 \sin\alpha\, \cos\alpha} \Bigg[& \int_{\mathrm{i}\infty}^{0} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(2)}(KR)\, \mathrm{d}\nu \\ & + 2\int_0^{\infty} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] J_\nu(KR)\, \mathrm{d}\nu \\ & + \int_{-\mathrm{i}\infty}^{0} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(1)}(KR)\, \mathrm{d}\nu \Bigg] \end{aligned} \tag{41}$$

which is the sum of three well-defined integrals. This representation results from (40) and the relation

$$J_\nu(KR) = \frac{1}{2}\left[H_\nu^{(1)}(KR) + H_\nu^{(2)}(KR)\right] \tag{42}$$

on the part of the contour where ν is real.

To prove that the solution (40) is equivalent to the function given by equation (31) we prove (a) that it is regular for $R \to 0$, (b) that it vanishes when $R \to \infty$ and $\alpha = \text{const}$, and (c) that it has the correct asymptotic behaviour (31) when $R \to \infty$ with $\alpha \to 0$ ($R\alpha = \text{const}$). This suffices to prove the equivalence of the two functions since they both satisfy the same Schrödinger equation, are regular everywhere and satisfy the same boundary conditions on a closed surface at infinity.

We first show that (40) is regular when $R \to 0$. To do that, we can take the limit $R \to 0$ underneath the integrals of (40) since the sum of the three integrals is convergent. In that way

we get

$$\tilde{\Psi}^{(1)}(\alpha, R) = \frac{1}{\mathrm{i}\pi}\frac{1}{R^2 \sin\alpha\, \cos\alpha}\left[-\int_{C_1} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]\Gamma(\nu)\left(\frac{1}{2}KR\right)^{-\nu} \mathrm{d}\nu \right.$$
$$\left. + \int_{C_2} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]\Gamma(\nu)\left(\frac{1}{2}KR\right)^{-\nu} \mathrm{d}\nu\right]. \tag{43}$$

It is apparent that the integrals corresponding to the real part of the contours C_1 and C_2 cancel. The remaining integral from $-\mathrm{i}\infty$ to $\mathrm{i}\infty$ can be evaluated using the residue theorem. Closing the contour to form a (counterclockwise) semicircular region bounded by $-\mathrm{i}\infty$ and $\mathrm{i}\infty$ over the left side of the plane ν we get contributions from the poles at $\nu = -n$ of the gamma function appearing in equation (43). For R small enough the only contribution due to the pole at $\nu = 0$ contributes, but at this point the pseudo-Sturmian function vanishes and the function reduces to order R^1. This analysis can also be done for general solutions of the TTRR assuming that there are no poles at $\mathrm{Re}[\nu] = 0$.

To show that (40) vanishes when $R \to \infty$ and $\alpha = \text{const}$ we replace the Bessel functions $H_\nu^{(1)}(KR)$ and $H_\nu^{(2)}(KR)$ by their limit expressions (for $R \to \infty$) under the sign of the integral. Again, this can be done because the integrals converge. Here it is essential that we make this replacement in all terms simultaneously. Thus we get

$$\tilde{\Psi}^{(1)}(\alpha, R) = \frac{\sqrt{\frac{2}{\pi K}}}{R^{5/2}\sin\alpha\, \cos\alpha}\left[\mathrm{e}^{-\mathrm{i}(KR-\frac{\pi}{4})}\int_{C_1} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\nu}\,\mathrm{d}\nu \right.$$
$$\left. + \mathrm{e}^{\mathrm{i}(KR-\frac{\pi}{4})}\int_{C_2} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\nu}\,\mathrm{d}\nu\right]. \tag{44}$$

Each of these integrals is evaluated using Cauchy's theorem. For example, we close the contour C_1 by joining the point ν_N (ν_N large) with the point $\mathrm{i}\infty$. The residue theorem ensures that the integral in the upper plane vanishes since there are no poles inside the contour. A completely similar procedure is used to evaluate the integral over contour C_2. In this way we prove that the integral representation given by equation (40) vanishes when $R \to \infty$ with α fixed. Note here that the contours can be closed only after substituting the asymptotic expressions for the Bessel functions.

It remains to prove point (c), namely, that the function (41) has the correct asymptotic behaviour when r_1 is fixed and $r_2 \to \infty$ or equivalently $R \to \infty$, $\alpha \to 0$ ($R\alpha = \text{const}$). To do that we will work with each of the integrals of equation (40) individually but with the understanding that the limits are always taken on the sum.

We consider the first integral of equation (40), namely

$$\psi_I(\alpha, R) = \int_{C_1} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right] H_\nu^{(2)}(KR)\,\mathrm{d}\nu \tag{45}$$

and use the stationary phase method to extract the asymptotic behaviour. Introducing the definitions $\nu = \mathrm{i}\mu R$ and $\alpha = r/R$ in equation (45) we get

$$\psi_I(\alpha, R) = \mathrm{i}\,R\int_{C_1} \mathrm{e}^{-\mathrm{i}\alpha_k\mu R} \sin\left[\mathrm{i}\mu R\left(\frac{\pi}{2}-\frac{r}{R}\right)\right] H_{\mathrm{i}\mu R}^{(2)}(KR)\,\mathrm{d}\mu. \tag{46}$$

For large R we use the asymptotic expression for $H_\nu^{(2)}(KR)$ from [16]:

$$H_\nu^{(2)}(KR) = \sqrt{\frac{2}{\pi R}}\frac{1}{\left[K^2-\frac{\nu^2}{R^2}\right]^{1/4}}\exp\left\{\mathrm{i}\int^{\nu}\arccos\left(\frac{\nu'}{KR}\right)\mathrm{d}\nu' + \mathrm{i}\frac{\pi}{4}\right\}. \tag{47}$$

It is straightforward to see that the stationary phase point is

$$\mu_0 = K \sinh(\alpha_k) = \tfrac{1}{a} \tag{48}$$

and the stationary phase value of the integral (46) is

$$\psi_I(\alpha, R) = -\mathrm{i}\, \mathrm{e}^{-r/a - \mathrm{i}kR} \tag{49}$$

where k is given by $k = \sqrt{K^2 + \frac{1}{a^2}}$.

Following the same procedure to study the function

$$\psi_{II}(\alpha, R) = \int_{C_2} \mathrm{e}^{-\nu\alpha_k} \sin\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(1)}(KR)\, \mathrm{d}\nu \tag{50}$$

we find that the asymptotic behaviour is given by

$$\psi_{II}(\alpha, R) \approx \mathrm{i}\mathrm{e}^{-r/a + \mathrm{i}kR}. \tag{51}$$

The linear combination of $\psi_I(\alpha, R)$ and $\psi_{II}(\alpha, R)$ defines $\tilde{\Psi}^{(1)}(\alpha, R)$. Using the results of equations (49) and (51) and introducing the normalization constant $A = -\frac{1}{2\sqrt{K}}$ we find

$$\tilde{\Psi}^{(1)}(\alpha, R) \approx \frac{\mathrm{e}^{-r_1/a}}{r_1} \frac{\sin(kR)}{R} \qquad R \to \infty \tag{52}$$

in agreement with the asymptotic form of (31). Because $\tilde{\Psi}^{(1)}(\alpha, R)$ of equation (40) and $\Psi^{(1)}(\alpha, R)$ are regular functions satisfying the same Schrödinger equation (16) and the boundary condition (18) on a closed surface, they are identical.

A completely similar analysis can be done with the function

$$\begin{aligned}\tilde{\Psi}^{(2)}(\alpha, R) = \frac{1}{R^2 \sin\alpha\, \cos\alpha} \Bigg[&\int_{C_1} \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(2)}(KR)\, \mathrm{d}\nu \\ &+ \int_{C_2} \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(1)}(KR)\, \mathrm{d}\nu \Bigg].\end{aligned} \tag{53}$$

Equation (53) is the generalized KL for the irregular wavefunction (32). The contours $C_{1,2}$ are described at the beginning of this section (see figure 1) and the same limit procedure should be understood. The regular representation similar to equation (41) is

$$\begin{aligned}\tilde{\Psi}^{()}(\alpha, R) = \frac{1}{R^2 \sin\alpha \cos\alpha} \Bigg[&\int_{\mathrm{i}\infty}^{0} \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(2)}(KR)\, \mathrm{d}\nu \\ &+ 2\int_{0}^{\infty} \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] J_\nu(KR)\, \mathrm{d}\nu \\ &+ \int_{-\mathrm{i}\infty}^{0} \mathrm{e}^{-\nu\alpha_k} \cos\left[\nu\left(\frac{\pi}{2} - \alpha\right)\right] H_\nu^{(1)}(KR)\, \mathrm{d}\nu \Bigg].\end{aligned} \tag{54}$$

The functions $\tilde{\Psi}^{(2)}(\alpha, R)$ and $\Psi^{(2)}(\alpha, R)$ are equivalent.

Equations (41) and (45) are the main results of this paper. The integral expression that we have obtained for $E > 0$ is unexpected, especially when compared with the standard expression that was easily found for $E < 0$. Yet we know that the solutions in Jacobi coordinates show no such dramatic difference in crossing the $E = 0$ threshold. To complete our analysis, we resolve this apparent contradiction and connect the expression for $E > 0$ to that for $E < 0$.

4.3. A connection between the representations

The function $\Psi^{(1)}(\alpha, R)$ of equation (31) is written in hyperspherical coordinates as

$$2\mathrm{i}\,\mathrm{e}^{-r_1/a}\sin(kr_2) = \mathrm{e}^{\mathrm{i}KR\cos(\alpha-\mathrm{i}\alpha_k)} - \mathrm{e}^{-\mathrm{i}KR\cos(\alpha+\mathrm{i}\alpha_k)} \tag{55}$$

where

$$\sinh\alpha_k = \frac{1/a}{\sqrt{k^2-1/a^2}} \qquad \cosh\alpha_k = \frac{k}{\sqrt{k^2-1/a^2}}. \tag{56}$$

Two different analytic continuations of the right-hand side can be used, namely

$$K = \mathrm{i}\mathcal{K} \qquad \alpha_k \to \alpha_k - \mathrm{i}\tfrac{\pi}{2} \tag{57}$$

and

$$K = -\mathrm{i}\mathcal{K} \qquad \alpha_k \to \alpha_k + \mathrm{i}\tfrac{\pi}{2}. \tag{58}$$

Both continuations of equation (55) give identical expressions,

$$2\mathrm{i}\,\mathrm{e}^{-r_1/a}\sin(kr_2) = \mathrm{e}^{-\mathcal{K}R\sin(\alpha-\mathrm{i}\alpha_k)} - \mathrm{e}^{-\mathcal{K}R\sin(\alpha+\mathrm{i}\alpha_k)}. \tag{59}$$

This means that there are two different ways to perform the analytic continuation in hyperspherical coordinates. The two ways are a consequence of using two 'coordinates' K and α_k to represent one variable k.

We now substitute equation (57) into the integral over C_1 and equation (58) into the integral over C_2 in equation (40) to obtain

$$\Psi^{(1)}(\alpha, R) = \frac{2}{\pi\mathrm{i}}\frac{1}{R^2\sin\alpha\,\cos\alpha}\left[\int_{-C_1}\mathrm{e}^{-\nu\left(\alpha_k-\mathrm{i}\frac{\pi}{2}\right)}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]H_\nu^{(2)}(\mathrm{i}\mathcal{K}R)\,\mathrm{d}\nu\right.$$
$$\left. + \int_{C_2}\mathrm{e}^{-\nu\left(\alpha_k+\mathrm{i}\frac{\pi}{2}\right)}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]H_\nu^{(1)}(-\mathrm{i}\mathcal{K}R)\,\mathrm{d}\nu\right]. \tag{60}$$

Introducing the connection between the Hankel functions $H_\nu^{(1,2)}$ and the Bessel function K_ν gives

$$\Psi^{(1)}(\alpha, R) = \frac{2}{\pi\mathrm{i}}\frac{1}{R^2\sin\alpha\,\cos\alpha}\left[\int_{-C_1}\mathrm{e}^{-\alpha_k\nu}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}\nu\right.$$
$$\left. + \int_{C_2}\mathrm{e}^{-\alpha_k\nu}\sin\left[\nu\left(\frac{\pi}{2}-\alpha\right)\right]K_\nu(\mathcal{K}R)\,\mathrm{d}\nu\right] \tag{61}$$

where $-C_1$ indicates a change of direction on the contour C_1.

It is readily apparent that the integrals over the real axis of ν cancel leaving only one integral along the imaginary axis from $\nu = -\mathrm{i}\infty$ to $\nu = \mathrm{i}\infty$. This is exactly the representation given by equation (38).

This shows us how the integral representations for E greater and less than zero are connected, even though the representations look very different. Two different analytic continuations lead to the same function for $E < 0$ in Jacobi coordinates. Nevertheless, we need both to continue the integral representation of equation (41). Only the correct combinations of the two continuations lead to the proper analytic extension.

5. Conclusions and remarks

In this paper we have considered the wavefunction for three particles when two of them interact via ZRPs. In the first place, we have written the exact solution using the representation introduced by Macek and Ovchinnikov for the Coulomb problem [3]. The case where all three

particles interact via ZRPs can be solved following the steps delineated in this work. Only a different expression for $\rho(\nu)$ is needed [6]

Two different kinds of pseudo-Sturmian functions $S(\nu, \alpha)$ for ZRPs have been introduced, discussed and applied. One of them is regular at $\alpha = \pi/2$ and the second has its derivative with respect to α regular at that point. From the physical point of view only the first solution seems to be of interest. Nevertheless, the second one is appropriate for the irregular solution.

The general solution using a Kontorovich–Lebedev-like representation was discussed in section 3. Once the pseudo-Sturmian and the radial functions were defined, the solution was written as a weighted integral of the product of those functions. The problem then reduces to a three-term recurrence relation for the weight function and to the determination of the integration contour. By choosing the solution of the TTRR and the contour properly, the Schrödinger equation and the boundary condition are satisfied.

Different KL representations were found for E greater and less than 0. For negative energies a traditional KL representation was found. However, a more elaborate representation was needed for positive energy. In that case the solutions were written as a sum of two integrals over the contours shown in figure 1. Two different Bessel functions are used to make the representation regular as a function of all the parameters and variables. This is one of the main contributions of this paper, namely we have found an alternative way to represent a function in terms of cylinder functions of an imaginary order. It could be understood as a generalization of the KL representation in the sense that the integrals are defined on a contour more general than the one introduced by Kontorovich and Lebedev. A connection between the representations for E greater and less than zero was also found.

The main new result of this work can be summarized by the equation

$$\int_0^\infty \left[\mathrm{e}^{-\nu\beta}\, J_\nu(\rho)\, \mathrm{d}\nu + \frac{1}{2}\mathrm{i}\, \mathrm{e}^{\mathrm{i}\nu\beta} H^{(1)}_{-\mathrm{i}\nu}(\rho) - \frac{1}{2}\mathrm{i}\, \mathrm{e}^{-\mathrm{i}\nu\beta} H^{(2)}_{\mathrm{i}\nu}(\rho) \right] \mathrm{d}\nu = \mathrm{e}^{-\rho \sinh\beta}. \tag{62}$$

It is a generalized KL representation for the function $\mathrm{e}^{-\rho\sinh\beta}$ where $\mathrm{Im}\,|\beta| < \frac{\pi}{2}$ and $\rho > 0$. This result cannot be found in standard tables, whereas the very similar expression of equation (35) can. Both expressions are needed to solve the Schrödinger equation for zero-range potentials in hyperspherical coordinates.

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