Scattering solutions of the spinless Salpeter equation

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A method to compute the scattering solutions of a spinless Salpeter equation (or a Schrödinger equation) with a central interaction is presented. This method relies on the three-dimensional Fourier grid Hamiltonian method used to compute bound states. It requires only the evaluation of the potential at equally spaced grid points and yields the radial part of the scattering solution at the same grid points. It can be easily extended to the case of coupled channel equations and to the case of nonlocal interactions. [S1063-651X(99)02701-4]

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I. INTRODUCTION

Numerous techniques have been developed to compute the scattering solutions of a Schrödinger equation. Simple Runge-Kutta methods can be performed in the case of a local potential and discretization of the integration domain can be used for a nonlocal interaction [1]. All these techniques can be used because the kinetic energy operator can be expressed in terms of a derivative operator. This is no longer true in the case of a spinless Salpeter equation for which the kinetic energy is a complicated square-root operator.

In a previous paper [2] we have developed a method to compute the eigenvalues of a spinless Salpeter equation. This method relies on the fact that the kinetic energy operator is best represented in momentum space, while the potential energy is generally given in coordinate space. It requires only the evaluation of the potential at equally spaced grid points and yields directly the amplitude of the solution at the same grid points. This method is derived from the Fourier grid Hamiltonian method [3,4] developed to compute the solution of the one-dimensional Schrödinger equation and consequently was called the three-dimensional Fourier grid Hamiltonian method. It appears very accurate and simple to handle.

In this paper we show that the three-dimensional Fourier grid Hamiltonian method can be used to compute the scattering solutions of a spinless Salpeter equation (or a Schrödinger equation). We focus our attention on the case of a purely central local potential, but the method can also be applied if the potential is nonlocal or if couplings exist between different channels. To our knowledge, this is the first time that the scattering solutions of the spinless Salpeter equation are presented.

Our method is outlined in Sec. II. Test applications of the method are presented in Sec. III. A brief summary is given in Sec. IV.

II. METHOD

A. Theory

We assume that the Hamiltonian can be written as the sum of the kinetic energy $\hat{T}$ and a potential energy operator $\hat{V}$. The scattering equation is given by

$$[\hat{T}+\hat{V}]|\Psi\rangle = E|\Psi\rangle, \tag{1}$$

where $\hat{T}$ depends only on the square of the relative impulsion $\vec{p}$ between the particles, $\hat{V}$ is a local interaction that depends on the relative distance, and E is the asymptotic kinetic energy of the two interacting particles. This equation is a spinless Salpeter equation if

$$\hat{T} = \sqrt{\vec{p}^2+m_1^2}+\sqrt{\vec{p}^2+m_2^2}-m_1-m_2, \tag{2}$$

where m_1 and m_2 are the masses of the particles (we use the natural units $\hbar = c = 1$ throughout the text). Equation (1) is a Schrödinger equation if

$$\hat{T} = \frac{\vec{p}^2}{2\mu} \quad \text{with} \quad \mu = \frac{m_1 m_2}{m_1+m_2}. \tag{3}$$

In configuration space, Eq. (1) is written

$$\int [\langle \vec{r}|\hat{T}|\vec{r}'\rangle + \langle \vec{r}|\hat{V}|\vec{r}'\rangle]\langle \vec{r}'|\Psi\rangle d\vec{r}' = E\langle \vec{r}|\Psi\rangle. \tag{4}$$

In the following, we consider only the case of a local central potential

$$\langle \vec{r}|\hat{V}|\vec{r}'\rangle = V(r)\,\delta(\vec{r}-\vec{r}') \quad \text{with} \quad r = |\vec{r}|. \tag{5}$$

Consequently, the wave function has the form

$$\langle \vec{r}|\Psi\rangle = R_l(r)\,Y_{lm}(\hat{r}) \quad \text{with} \quad \hat{r} = \vec{r}/r. \tag{6}$$

Using the method developed in Ref. [2], Eq. (4) can be rewritten as

$$\frac{2}{\pi} r \int_0^\infty dr' r' u_l(r') \int_0^\infty dq\; q^2 T(q^2) j_l(qr) j_l(qr') + V(r) u_l(r) = E u_l(r), \tag{7}$$

where $u_l(r) = rR_l(r)$ is the regularized radial function and the functions $j_l(qr)$ are spherical Bessel functions.

Using the orthogonality relation

$$\frac{2}{\pi} xx' \int_0^\infty j_l(qx) j_l(qx') q^2 dq = \delta(x-x'), \tag{8}$$

one can show that $u_l(r) \propto r j_l(kr)$, with k fixed, is a solution of Eq. (7) with vanishing potential. The relative energy E is

then equal to $\sqrt{k^2+m_1^2}+\sqrt{k^2+m_2^2}-m_1-m_2$ in the case of a spinless Salpeter equation and $k^2/2\mu$ in the case of a Schrödinger equation.

B. Discretization

In order to compute the scattering solutions of Eq. (7), we replace the continuous variable r by a grid of discrete values r_i defined by

$$r_i = i\Delta \quad \text{with} \quad i=0,1,\ldots,N, \tag{9}$$

where Δ is the uniform spacing between the grid points. Regularity at the origin $r_0=0$ imposes $u_l(r_0)=0$. In the following, we always consider a potential with a finite range $\lim_{r\to\infty} rV(r)=0$ (the case of scattering by a Coulomb-like potential is not considered here). Outside the range of the potential, the solution is a phase shifted free wave function. For a value of $r_N=N\Delta$ sufficiently large, we choose to set arbitrarily $u_l(r_N)=1$ in order to fix the normalization of the wave function.

As explained in Ref. [2], the spacing Δ in the configuration space determines the grid spacing Δk in the momentum space. Therefore, we have a grid in the configuration space and a corresponding grid in the momentum space

$$k_s = s\Delta k = \frac{s\pi}{N\Delta} \quad \text{with} \quad s=0,1,\ldots,N. \tag{10}$$

If we note that $V_i=V(r_i)$, the discretization procedure replaces the continuous equation (7) by a matrix equation

$$\sum_{j=1}^{N-1} [H_{ij}-E\delta_{ij}]\phi_j = -H_{iN} \quad \text{for} \quad i=1,\ldots,N-1, \tag{11}$$

where

$$H_{ij} = \frac{2\pi^2}{N^3} ij \sum_{s=1}^{N} s^2 T\left(\left(\frac{\pi s}{N\Delta}\right)^2\right) j_l\left(\frac{\pi}{N} si\right) j_l\left(\frac{\pi}{N} sj\right) + V_i\delta_{ij}. \tag{12}$$

The discrete solution ϕ_i of the linear system (11) gives approximately the values of the radial part of the solution of Eq. (7) at the grid points: $\phi_i \simeq u_l(r_i)$. The phase shift can be computed by using the values of the wave function at two points in the region where the potential is vanishing [5].

This method can also be used in the case of a nonlocal potential and in the case of coupled-channel calculations. Some details about the implementation of such problems are given in Ref. [2].

Actually, the scattering solution cannot be obtained directly from Eq. (11). For instance, in the case of a zero angular momentum solution, it is easy to see that $H_{iN}=0$. Consequently, we have to set $u_l(r_{N-1})=1$ and to restrict the summation in Eq. (11) to $N-2$ [the point $u_l(r_N)$ cannot be determined]. Other normalization problems appear for all values of angular momentum. All are due to the discretization procedure as explained below.

The three-dimensional Fourier grid Hamiltonian method relies on the relation (8). The equivalent discrete orthogonality relation on our grid of points is

$$\frac{2\pi^2}{N^3} ij \sum_{s=1}^{N} s^2 j_l\left(\frac{\pi}{N} si\right) j_l\left(\frac{\pi}{N} sj\right) = \Delta_{ij}^{(N,l)}. \tag{13}$$

One can thus expect that $\Delta_{ij}^{(N,l)}=\delta_{ij}$ for all values of N and l. Actually, the situation is less favorable. In Ref. [2] we show that, for $l=0$, we have

$$\Delta_{ij}^{(N,l=0)} = \delta_{ij} \quad \text{for} \quad i,j=1,\ldots,N-1. \tag{14}$$

We have verified numerically that

$$\lim_{N\to\infty} \Delta_{ij}^{(N,l=1)} = \delta_{ij} \quad \text{for} \quad i,j=1,\ldots,N-1, \tag{15a}$$

$$\lim_{N\to\infty} \Delta_{ij}^{(N,l>1)} \approx \delta_{ij} \quad \text{for} \quad i,j=1,\ldots,N-1. \tag{15b}$$

Consequently, the accuracy of this method becomes poorer when l increases; nevertheless, for large enough number of grid points, very good results can be obtained.

For scattering problems, it is also interesting to calculate the values of the $\Delta_{iN}^{(N,l)}$ quantity. One can also expect that $\Delta_{iN}^{(N,l)}=\delta_{iN}$ for all values of N and l. Actually, it is easy to show that

$$\Delta_{iN}^{(N,l=0)} = 0. \tag{16}$$

For other values of l, we have verified numerically that

$$\lim_{N\to\infty} \Delta_{iN}^{(N,l\neq 0)} = 0 \quad \text{for} \quad i=1,\ldots,N \quad \text{and} \quad l \quad \text{even}, \tag{17a}$$

$$\lim_{N\to\infty} \Delta_{iN}^{(N,l\neq 0)} = 2\delta_{iN} \quad \text{for} \quad i=1,\ldots,N \quad \text{and} \quad l \quad \text{odd}. \tag{17b}$$

The simple way to obtain a correct normalization for the solutions, that is to say, a value of 1 for the regularized radial part of the wave function at the last point of integration, is to solve two different linear systems with respect to the parity of the angular momentum. As we shall show in the next section, the following procedures allows us to obtain accurate solutions of the scattering problem:

$$\sum_{j=1}^{N-2} [H_{ij}-E\delta_{ij}]\phi_j = -H_{iN-1} \quad \text{for} \quad i=1,\ldots,N-2 \quad \text{and} \quad l \quad \text{even}, \tag{18a}$$

$$\sum_{j=1}^{N-1} [H_{ij}-E\delta_{ij}]\phi_j = -H_{iN}/2 \quad \text{for} \quad i=1,\ldots,N-1 \quad \text{and} \quad l \quad \text{odd}. \tag{18b}$$

III. NUMERICAL IMPLEMENTATION

A. Free solutions

As noted above, solutions of the nonrelativistic and semirelativistic free equation (7) can be expressed in terms of

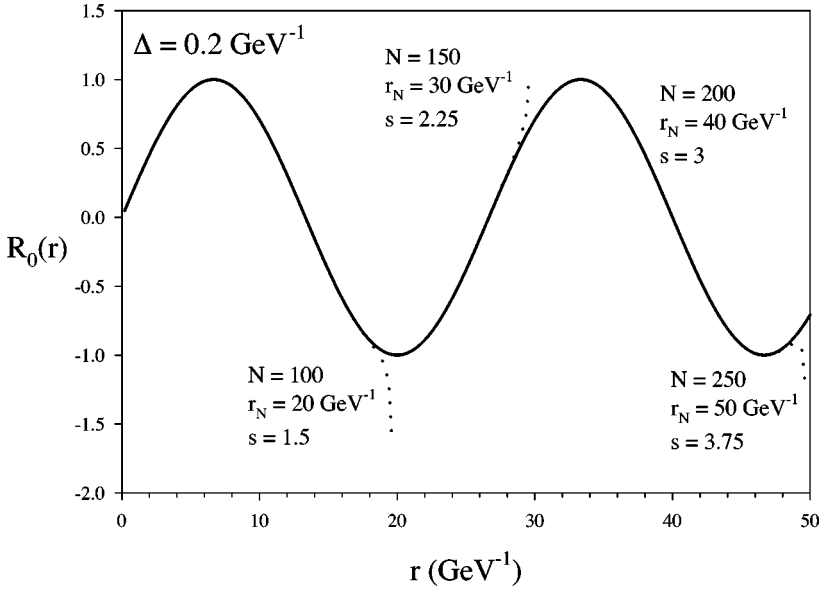

FIG. 1. Regularized radial part $R_0(r)$ of computed solutions (dotted lines) and the exact solution (solid line) for the semirelativistic free equation with a given relative kinetic energy and a zero angular momentum. The computed solutions are given for the same spacing, but for different values of r_N. The value of the parameter $s=N\Delta k/\pi$ is also presented. The energy is chosen in order that $s=3$ for $r_N=40$ GeV^{-1}. All computed wave functions are normalized to match the exact solution.

spherical Bessel functions. It can be easily shown that the vector $\{r_i j_0(kr_i);\ i=1,\ldots,N-2\}$, up to a normalization constant, is a solution of the system (18a) in the absence of a potential for $l=0$ if $k=(\pi/N\Delta)s$ with $s=1,\ldots,N-2$. This vector is no longer a solution if k is not a integer multiple of $\pi/N\Delta$. In this case the computed solution matches the solution of the continuous equation (7) everywhere, except near the last point r_N of the domain of integration. This situation is illustrated in Fig. 1 for the semirelativistic free equation. The regularized radial part of the computed solution for a given energy is presented for the same value of the spacing, but for different values of r_N. The relative kinetic energy being fixed, different values of r_N correspond to different values for the parameter s. We can show in this figure that the computed solutions differ from the exact solution when s is not an integer. The situation is not modified by a change of the energy.

If the angular momentum l is different from zero, then the vector $\{r_i j_l(kr_i)\}$ is not an exact solution of the system (18a) or (18b). Nevertheless, a very good approximation of the continuous free solution can be obtained with correct values for the parameters Δ and r_N. Again, the computed and the exact solutions can differ strongly near the last point r_N. It is worth noting that the differences between the computed and the exact solutions are much smaller in the nonrelativistic case, whatever the value of l.

In the free case, the phase shift is expected to be zero. Numerically, the phase shift can be determined by using two points of the computed solution. If these points are chosen in the region near r_N, the phase shift found can be different from zero. On the contrary, when the two points are taken far from r_N, the phase shift value vanishes.

B. Gaussian potential

We have tested our method with different finite range potentials in the case of symmetric or asymmetric systems. In this section we shall present only some results obtained with a Gaussian potential

$$V(r)=-V_0 e^{-r^2/a^2} \tag{19}$$

for two identical particles $m_1=m_2=m$.

In the free case, the computed solution can differ strongly from the real solution near the last point r_N. This is also the case when a potential is turned on. The phase shift can be computed with two values of the numerical solution evaluated at two different points r_p and r_q. If p or q is too close to N, then the value of the phase shift can be very bad. Obviously, the two points must be taken in a region where the potential can be neglected with respect to the relative kinetic energy. A good procedure to get a reliable phase shift is to compute the wave function with a large value of r_N. Then the phase shift can be computed with two adjacent points r_p and r_{p-1} as a function of the index p. By decreasing the value of p from N, the phase shifts will first strongly vary and rapidly reach a stable value, as long as r_p is large enough to not fall in a region where the potential cannot be neglected. This situation is illustrated in Fig. 2. In this figure the phase shift for two identical semirelativistic particles with $m=1$ GeV is plotted as a function of r_p for two values of the relative energy and for two values of r_N. The Gaussian potential is characterized by $V_0=0.5$ GeV and $a=10$ GeV^{-1}. It is worth noting that the variation of the phase shifts is much larger for the semirelativistic case than for the nonrelativistic case.

Scattering states have been calculated with our method for two nonrelativistic particles interacting with a Gaussian potential. In this case, wave functions and phases shifts can also be computed with a great variety of methods. For a large range of relative energy and for angular momentum varying from 0 to 4, we have checked that all approaches give the same results. Within our method, a relative accuracy of at least 10^{-4} for phase shifts can be obtained with a grid containing 200–400 points. Obviously, the interest of our method is to compute scattering solutions in the semirelativistic case.

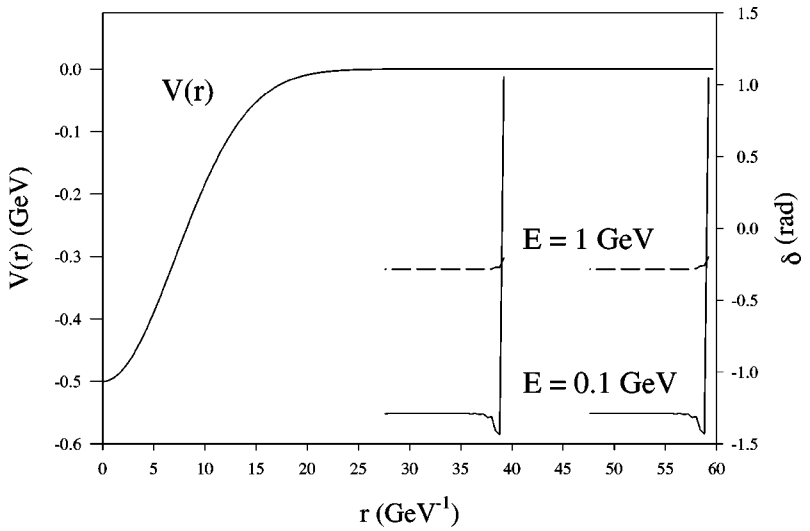

FIG. 2. Phase shifts δ in radians for two identical semirelativistic particles with $m=1$ GeV, interacting via a Gaussian potential with $V_0=0.5$ GeV and $a=10$ GeV^{-1}. The phase shifts are plotted as a function of r_p (see Sec. III B) for two values of the relative energy and for two values of r_N. The potential as a function of r is also indicated.

It is shown in the Appendix that a spinless Salpeter equation with a particular separable nonlocal potential can be transformed into a Schrödinger-like nonlocal equation. In this case, the scattering semirelativistic equation can be solved directly by the Fourier grid Hamiltonian method or using the equivalent Schrödinger-like form by the usual techniques. We have verified, for several values of the parameters and for different values of the relative kinetic energy, that all methods give the same results. This yields a direct verification of our approach.

Finally, we give, in Table I, the phase shifts for two identical particles interacting via a Gaussian potential as a function of the relative kinetic energy. Results have been computed for a nonrelativistic and a semirelativistic kinematics and for two values of the angular momentum l. As expected, phase shifts are similar for low relative energy and differ when energy increases.

TABLE I. Phase shifts for two identical particles with $m=1$ GeV as a function of the relative kinetic energy E. The interaction is a Gaussian potential with $V_0=0.1$ GeV and $a=5$ GeV^{-1} [see Eq. (19)]. Results are given for a nonrelativistic (NR) and a semirelativistic (SR) kinematics and for two values of the angular momentum l.

l	E (GeV)	δ_{NR} (rad)	δ_{SR} (rad)
0	0.001	−0.192	−0.189
	0.01	−0.627	−0.619
	0.1	1.363	1.376
	1	0.447	0.524
	10	0.156	0.256
1	0.001	−0.231	−0.226
	0.01	−0.931	−0.925
	0.1	1.241	1.254
	1	0.479	0.517
	10	0.156	0.256

IV. SUMMARY

The three-dimensional Fourier grid Hamiltonian method, used in a previous work to compute bound states [2], appears as a convenient method to find the scattering solutions of a spinless Salpeter equation (or a Schrödinger equation). It has the advantage of simplicity since it requires only the evaluation of the potential at some grid points and it generates directly the values of the radial part of the wave function at the same grid points. Moreover, the method can be extended to the cases of nonlocal interaction or coupled-channel equations. To our knowledge, this is the first time that the scattering solutions of the spinless Salpeter equation have been presented.

Meson-meson scattering has been recently investigated in terms of quark degrees of freedom within the framework of the nonrelativistic resonating group method [6]. From this work it appears that the use of a semirelativistic kinematics is necessary to avoid inconsistencies related to the nonrelativistic formalism. We have calculated a semirelativistic version of the pion-pion scattering equation. This equation is a scattering spinless Salpeter equation. In this framework, the method presented here appears suitable to calculate the corresponding phase shifts [7].

The accuracy of the solutions of the numerical method presented here can easily be controlled since it depends only on two parameters: the number of grid points and the largest value of the radial distance considered to perform the calculation. This distance must be large enough to fall in the region where the potential can be neglected with respect to the asymptotic kinetic energy. Both parameters can be automatically increased until a convergence is reached for phase shifts.

The method involves the use of matrices of order $N\times N$, where N is the number of grid points. Generally, the most time consuming part of the method is the solution of the linear system. This is not a problem for modern computers, even for personal computer stations. Moreover, several powerful techniques exist and can be used conveniently [10].

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APPENDIX: PARTICULAR CASE OF THE SPINLESS SALPETER EQUATION

The spinless Salpeter equation for two identical particles interacting via a nonlocal potential can be written

$$2\sqrt{\vec{p}^2+m^2}\,\Psi(\vec{r})=M\Psi(\vec{r})-\int d\vec{r}\,' W(\vec{r},\vec{r}\,')\Psi(\vec{r}\,'). \tag{A1}$$

Acting on both sides with the square-root operator gives

$$4(\vec{p}^2+m^2)\Psi(\vec{r})=M\left(M\Psi(\vec{r})-\int d\vec{r}\,' W(\vec{r},\vec{r}\,')\Psi(\vec{r}\,')\right) -2\int d\vec{r}\,'\sqrt{\vec{p}^2+m^2}\,W(\vec{r},\vec{r}\,')\Psi(\vec{r}\,'). \tag{A2}$$

If the potential has the form $W(\vec{r},\vec{r}\,')=V_0V(r)V(r')$ and if we perform the integrations on angular variables, we obtain

$$\left(\vec{p}^2+m^2-\frac{M^2}{4}\right)R_0(r)=-\pi V_0(M+2\sqrt{\vec{p}^2+m^2}) \times V(r)\int_0^\infty dr'r'^2V(r')R_0(r'), \tag{A3}$$

where $R_0(r)$ is the radial part of the S-wave function $\Psi(\vec{r})$. It has been shown in Ref. [8] that

$$\sqrt{\vec{p}^2+m^2}\,e^{-mr}=\frac{4m}{\pi}K_0(mr), \tag{A4}$$

where $K_0(x)$ is a modified Bessel function (see [9], p. 952). In this case, if we choose $V(r)=\exp(-mr)$, then Eq. (A1) reduces to a nonlocal Schrödinger-like equation

$$\left(\frac{d^2}{dr^2}-m^2+\frac{M^2}{4}\right)u_0(r)=V_0(M\pi e^{-mr}+8mK_0(mr)) \times r\int_0^\infty dr'r'e^{-mr'}u_0(r'), \tag{A5}$$

where $u_0(r')=r'R_0(r')$.

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