New approach to numerical computation of the eigenfunctions of the continuous spectrum of three-particle Schrödinger operator: I. One-dimensional particles, short-range pair potentials

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Received 26 September 2009, in final form 10 May 2010
Published 16 June 2010
Online at stacks.iop.org/JPhysA/43/285205

Abstract
We use analogy between the three-body scattering problem and the diffraction problem of the plane wave by a system of semi-transparent half screens, and propose a new approach to the few-body scattering problem. The numerical results have been obtained for the case of the short-range non-negative pair potentials. The developed method allows a natural generalization to the case of long-range pair potentials.

PACS numbers: 03.65.Nk, 31.15.ac
Mathematics Subject Classification: 34L25, 81U08

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In this work we consider only the quantum system of three particles with short-range pair potentials, but our distant goal is to develop a systematic approach to the systems of charged particles, i.e. particles with long-range pair interactions. The quantum system of two particles interacting via the Coulomb potential is probably the most known model of quantum mechanics. The model allows an explicit solution. On the contrary, the mathematical status of the system of three quantum particles with the pair Coulomb interaction is relatively poor. The system of three particles with short-range pair interactions was successfully studied by Faddeev [1], but the direct generalization to the Coulomb-type potentials was found to be impossible. Something, however, is known: the quantitative nature of the spectrum and the large time asymptotic behavior of the solutions of the non-stationary Schrödinger equation. These results were obtained in frameworks of a non-stationary approach, see [2, 3]. Nevertheless, a mathematically consistent stationary approach similar to the Lippmann–Schwinger integral
equation, or something analogous (see, for example, [4]), has not been developed yet. Such an approach is needed if we are interested in numerical parameters of many important physical processes like dissociative recombination in atomic and molecular physics with applications to astrophysics, medicine, chemical physics, etc.

There are specific difficulties that are characteristic for systems with Coulomb-type interactions.

They are naturally explained by the fact that the long-range interactions crucially affect the asymptotic behavior at infinity in the configuration space of the eigenfunctions, Green’s functions and other similar objects. The consequences of that influence on the structure of asymptotic behavior have not been taken in account in a correct mathematical manner until now. As a result, such approaches to many particle scattering as Faddeev’s equations [1] and AGS equations [6], successfully applicable to the systems with short-range potentials, do not work for the systems with the long-range potentials.

These difficulties were discovered in the work by Dollard [7] who also proposed a way of regularization of the wave operators for the case of the Coulomb-type interaction. More general long-range potentials were considered later in [8]; here also the elements of stationary regularization were proposed.

The asymptotic behavior of the wavefunctions for the systems of few charged particles has been studied only in some domains of configuration space but not for all asymptotic directions. Let us shortly list some known results. In [9, 10] the asymptotic behavior of three charged particles’ wavefunction for the case of large distances between all three particles was studied. Another limiting case, considered in [11], corresponds to configurations where one Jacobi coordinate is much larger than another.

In the list of literature addressing the theoretical aspects of the problem we also mention [13–19]. Applications to the computational aspects of the problem were treated in [20–26].

One of the most typical computational approaches to such systems is the replacement of the Coulomb potentials by the Yukava potentials (or some other cutoff potentials), further computation of the parameters of scattering for such a modified system, and considering the results for small screening parameter. Mathematically, it is not a completely satisfactory procedure.

Recall that although the distant goal of the project is improvement of the stationary approach to the system of three charged particles, in this work we consider only the case of short-range potentials. However, we could already see that the results of the present work are crucially important for their generalization to the case of long-range potentials.

We assume here that the pair potentials are non-negative. In this case the spectrum is purely continuous, covers the positive semi-axis and is in the natural sense homogeneous. In fact, this case is the most interesting at the present stage since the lower spectral branches for negative total energy in the case of charged particles were already treated in [31].

It is worth mentioning that the scattering in the system of one-dimensional particles also provides a way towards studying the case of three-dimensional particles. It is interesting in itself that the systems of three one-dimensional particles (neutral or charged) were intensively studied for many years (see, for example, [32–36]). In recent years there appeared a new interest to such systems since they were realized experimentally (see [37–40]).

The main idea is to suggest, may be not rigorously justified, but explicit formulas for the asymptotic behavior of the eigenfunctions of the continuous spectrum.

The formulas describe the eigenfunctions at infinity in the configuration space up to the simple diverging waves with smooth amplitudes. If we are able to find such asymptotic behavior (satisfying certain criteria that will be discussed later on) even heuristically, we obtain a way for regular numerical computations of the eigenfunctions. We also obtain
simultaneously a method to construct an appropriate integral equation of the same nature as the Lippmann–Schwinger equation for the scattering of the plane wave by a quickly decreasing potential that can be used to justify the asymptotic behavior rigorously following the ideas of [5].

For one-dimensional particles with quickly decreasing pair potentials at infinity we can use, for the description of the mentioned asymptotic behavior, the analogy between the stated problem and the classical problem of the diffraction of the plane waves by the set of semi-transparent infinite screens. This analogy was already used in [27–30]. In the case of long-range potentials we hope to be able to treat the diffraction problem analogously with the replacement of the classical plane waves by plane waves that are appropriately deformed by the long-range tails of the Coulomb potentials. It is important to mention that the diffraction itself and the corresponding scattering problems cannot be completely reduced to the scattering of the plane waves by the screens; we have to add to these processes some genuine diffraction components that have a more complicated analytical structure but still an explicit description. This more complicated structure is also dictated by the analogy with the classical diffraction theory.

Here we consider a system of three identical one-dimensional quantum particles interacting via short-range pair potentials. In the following publications we consequentially will remove these limitations. As we have mentioned above, the theoretical part of this work is already published [30], but we decided for completeness to repeat briefly the main theoretical ideas here. The main goal of this paper is to confirm that the approach works for the numerical computation of the eigenfunctions of the continuous spectrum. The approach is new even for the short-range pair potentials.

The structure of the work is as follows: it consists of two parts. The first part is devoted to the theoretical constructions. The second part is original and represents the results of numerical computations.

2. Main formulas

2.1. Configuration plane

We consider a quantum system of three particles on the axis. Let us denote by $v(x)$, $x \in \mathbb{R}$, the potential of the pair interaction; then we suppose that it is a real-valued smooth even function with compact support, $v(x) = 0$, $|x| > h/2$. In the system of three particles we can separate three subsystems of two particles: let us numerate them by $j, j = 1, 2, 3$.

The original configuration space of the system is the Euclidian space $\mathbb{R}^3$ of points $z = (z_1, z_2, z_3)$. Let us put $\sqrt{2} x_1 = z_3 - z_2$, geometrically; this is the difference of the coordinates of particles in the pair $j = 1$. Using cyclic permutation we can define $x_2, x_3$ analogously. Note that $x_1 + x_2 + x_3 = 0$.

The configuration space of the system after the separation of motion of the center of mass is the hyperplane $\Gamma = \{z = (z_1, z_2, z_3) : z_1 + z_2 + z_3 = 0\}$ in $\mathbb{R}^3$.

As independent coordinates we can use on $\Gamma$ three coordinates $x_1, x_2, x_3$ satisfying the condition $x_1 + x_2 + x_3 = 0$. We also can consider three pairs of the Jacobi coordinates $(x_j, y_j)$, $y_j = \sqrt{\frac{2}{3}} z_j$.

The standard scalar product on $\Gamma$ can be described by the following formulas:

\[
(q, z) = q_1 z_1 + q_2 z_2 + q_3 z_3 = \frac{2}{3} (k_1 x_1 + k_2 x_2 + k_3 x_3) = p_j y_j + k_j x_j, \quad j = 1, 2, 3. \tag{1}
\]

In these formulas $q, z$ are two vectors of $\Gamma$ with the original coordinates $(q_1, q_2, q_3), (z_1, z_2, z_3)$. By $x_j, k_j$ we denote their first Jacobi coordinates, and, at last, $(x_j, y_j), (k_j, p_j)$ are the Jacobi coordinates of $z, q$. 


The Schrödinger equation for the system on $\Gamma$ after the appropriate choice of the units and with appropriate normalization of the potential takes the form

$$- \Delta \psi + (v(x_1) + v(x_2) + v(x_3))\psi = E\psi, \tag{2}$$

where $\psi = \psi(z) \in C$, $\Delta$ is the Laplace operator on $\Gamma$. In Jacobi coordinates it can be described by the standard expression

$$\Delta = \frac{\partial^2}{\partial y_j^2} + \frac{\partial^2}{\partial x_j^2}. \tag{3}$$

Let us consider on $\Gamma$ three straight lines $l_j = \{x : x_j = 0\}$, $j = 1, 2, 3$, and three unit vectors $l_j$ that belong to these lines and oriented such that $x_{j+1}$ increases along $l_j$. Also consider the unit vectors $k_j$ that are orthogonal to $l_j$ and oriented along the direction of increasing of $x_j$.

The lines $l_j$ define on the plane $\Gamma$ six sectors. The internal part of a certain one consists of the vectors $(x_1, x_2, x_3)$ whose coordinates satisfy the condition $x_{j_1} > x_{j_2} > x_{j_3}$ where $\sigma = (j_1, j_2, j_3)$ is a permutation of the numbers $(123)$. We will denote any sector by the corresponding permutation $\sigma$ and will write $\lambda = \lambda_\sigma$ (see figure 1).

Let the group $S_3$ of permutation acts on $\Gamma$ so that

$$ (\sigma, x) \rightarrow \sigma x = (x_{j_1}, x_{j_2}, x_{j_3}), \quad \sigma = (j_1, j_2, j_3), \quad x = (x_1, x_2, x_3).$$

The group contains six elements. The permutation can be identical, or a transposition of two elements, or a composition of two transpositions, some of the compositions coincide. Introduce the notations for the transpositions: $\tau_1 = (132)$, $\tau_2 = (321)$, $\tau_3 = (213)$, and note that $\tau_i^2 = I$, $i = 1, 2, 3$. The action of the transposition on $\Gamma$ will be denoted by the same symbol $\tau_j$, $j = 1, 2, 3$. It corresponds to the reflection with respect to the line $l_j$, $j = 1, 2, 3$.

It is clear that

$$\tau_1(x_1, x_2, x_3) = (-x_1, -x_3, -x_2), \tag{4}$$

the analogous formulas are also satisfied for $\tau_2, \tau_3$. The composition of two transpositions generates a rotation, and the following equalities, in particular, hold: $\tau_1 \tau_2 = \tau_3 \tau_1 = \tau_2 \tau_3$, $\tau_2 \tau_1 = \tau_1 \tau_3 = \tau_3 \tau_2$.

Let $q$ be a vector that does not belong to any $l_j$, $j = 1, 2, 3$. Six elements $r$ of the group $S_3$ generate six vectors $r q$. If $q \in \lambda_\sigma$, then $r q \in \lambda_{r \sigma}$, see figure 1.
2.2. Separation of variables

Consider now the eigenfunction that describes the scattering in the system where just one of the three potentials is not equal to zero. Now we deal with the Schrödinger equation

$$-\Delta \chi_j + v(x_j) \chi_j = E \chi_j.$$  

(5)

It allows the separation of variables

$$\chi_j (z, q) = \chi(x_j, k_j) e^{i p_j y_j}.$$  

(6)

The sense of the variables \((x_j, y_j)\) is clear and \((k_j, p_j)\) are the Jacobi coordinates of the given vector \(q\).

The function \(\chi(x, k)\), \(x, k \in \mathbb{R}\), is a solution of the ordinary differential equation

$$-\chi_{xx} + v(x) \chi = k^2 \chi,$$  

(7)

which has to be described separately. For \(k > 0\) there exists a unique solution that is characterized by the following asymptotic behavior:

$$\chi(x, k) \sim s(k) e^{ikx}, \quad x \to +\infty; \quad \chi(x, k) \sim e^{ikx} + r(k) e^{-ikx}, \quad x \to -\infty.$$  

(8)

To the whole axis \(k\) this solution, due to the evenness of the potential, has to be extended by the formula

$$\chi(x, k) = \chi(-x, -k).$$

Here \(s\) and \(r\) are some complex-valued functions of \(k\) that are called the transition and the reflection coefficients.

We assumed earlier that \(v(x) \geq 0\); therefore, equation (7) does not have the bound states.

2.3. Formal setting of the problem

Our final goal is to construct the solution \(\psi(z, q)\) of the Schrödinger equation on \(\Gamma\) that is characterized by the following behavior at infinity:

$$\psi = n(z, q) e^{-i|z||q|}/|z|^{1/2} + f(z, q) e^{i|z||q|}/|z|^{1/2} + o\left(\frac{1}{|z|^{1/2}}\right), \quad \hat{z} = \frac{z}{|z|}.$$  

(9)

Here

$$n(z, q) = \sqrt{\frac{2\pi}{i|q|}} \delta(\hat{z}, \hat{q})$$  

(10)

and the \(\delta\) function has to be considered with respect to the angle measure on the unit circle.

Sometimes we will call such solutions scattered plane waves (corresponding to the wave vector \(q\)). They are the generalized eigenfunctions of the continuous spectrum.

The asymptotic behavior has to be treated in a weak sense (in the sense of distributions) with respect to \(\hat{z}\). The coefficient \(n\) before the converging circle wave coincides with the analogous coefficient before the converging wave in the weak asymptotic representation of the plane wave \(e^{i\varphi}q^0\).

Due to the symmetries of the potential \(\psi(z, q) = \psi(\sigma z, \sigma q), \sigma \in S\), we can always assume that \(q\) belongs to a certain sector and we already selected it as \(\lambda_1 \equiv \lambda_{123}\). Earlier we restricted ourselves by the assumption that \(q\) does not belong to neighborhoods of the boundaries of the sector, it would not be hard to consider also the case when \(q\) belongs to the lines \(l_j\) and their neighborhoods.

The function \(f\) is a singular distribution. We will see that it has singularities on all six directions \(\sigma q, \sigma \in S\). Four of them are of \(\delta\)-function type, and two (for \(\sigma q = \tau_2 \tau_3 q, \tau_2 \tau_1 q\)) are of the type of Cauchy’s limiting kernel. It is worth noting that although the asymptotic behavior is singular the solution itself is, naturally, a smooth function.
In the case of the scattering by a potential quickly decreasing at infinity, the asymptotic behavior is given by the formula
\[ \psi(z, q) = e^{i\langle z, q \rangle} + f(\hat{z}, q) \frac{e^{i|z||q|}}{|z|^{1/2}} + o\left(\frac{1}{|z|^{1/2}}\right), \tag{11} \]
where that time the scattering amplitude \( f \) is not a singular distribution, but a smooth function, and the asymptotic behavior, can be treated in a uniform sense.

Under our assumptions over the potential the scattered plane waves create for \( E > 0 \) a complete system of the eigenfunctions of the continuous spectrum of the three-particle Schrödinger operator, \( E \geq 0 \).

Our further plan is as follows: we construct in explicit form a function \( \psi_1(z, q) \) and hope that the difference \( \psi - \psi_1 \) has the diverging asymptotic behavior
\[ \psi(z, q) - \psi_1(z, q) = g(\hat{z}, q) \frac{e^{i|z||q|}}{|z|^{1/2}} + o\left(\frac{1}{|z|^{1/2}}\right), \tag{12} \]
where \( g \) is a continuous function of the arguments.

Constructing \( \psi_1 \) we use two criteria: (1) the discrepancy \( Q[\psi_1](z, q) = -\Delta \psi_1 + (v(x_1) + v(x_2) + v(x_3))\psi_1 - E\psi_1, \quad E = |q|^2 \) sufficiently quickly vanishes at infinity and (2) the asymptotic representation for \( \psi_1 - e^{i\langle z, q \rangle} \) contains asymptotically only the diverging wave.

Consider the difference
\[ \xi = \psi - \psi_1. \tag{14} \]
It satisfies the equation
\[ H\xi - E\xi = -Q, \quad H = -\Delta + (v(x_1) + v(x_2) + v(x_3)). \tag{15} \]
Since \( Q \) is quickly vanishing one can hope that \( \xi \) asymptotically behaves as the diverging wave
\[ \xi(z, q) = g(\hat{z}, q) \frac{e^{i|z||q|}}{|z|^{1/2}} + o\left(\frac{1}{|z|^{1/2}}\right), \tag{16} \]
with a continuous amplitude \( g \). In other words, \( \xi \) satisfies the classical radiation conditions at infinity.

All these results are justified here and in [28] only heuristically. But with these heuristical results supported now by the numerical computations we firmly believe that mathematically rigorous justification of the proposed asymptotic formulas for the generalized eigenfunctions can also be given. It is natural to hope that for \( \xi \) we can construct an integral equation with the same properties as the properties of the classical Lippmann–Schwinger equation. We can do it by developing the ideas of work [5]. But we decided to postpone the development of this plan, and continue to study heuristically the asymptotic behavior of the scattered plane waves for the case of the Coulomb-type pair potentials.

Since it turned out possible to combine this work with numerical computations, we decided to apply the formulas of [28] and this work to the computations of the scattered plane wave. The report is also presented here. We use for the computation of \( \psi \) the problem (15) and (16) for \( \xi \). For the numerical computations we can replace (16) by the approximate boundary condition
\[ \left( \frac{\partial}{\partial |z|} - i\sqrt{E} \right) \xi = 0, \quad \text{for } |z| = R, \tag{17} \]
where \( R \) is sufficiently large.
The following construction of \( \psi_1 \) will consist of two steps. First, we construct for \( \psi_1 \) the so-called ray approximation \( \psi_R \). Its discrepancy has some singularities. After a natural modification motivated by some classical diffraction problems the discrepancy will become a smooth function.

2.4. Ray approximation

We already have fixed a vector \( \mathbf{q} \), \( \mathbf{q} \not\in \mathbf{l}_j \), \( j = 1, 2, 3 \), and introduced six vectors \( \sigma \mathbf{q} \). These vectors, more precisely, the rays containing them, define on \( \Gamma \) six sectors that we denote by \( K_j^\pm \). The indices of the notation coincide with the indices \( \pm \) of the vector \( \pm \mathbf{l}_j \) that belongs to the sector \( K_j^\pm \).

Now we can give explicit expressions for the ray approximation in different sectors \( K_j^\pm \).

Sector \( K_j^\pm \): \( \psi_R = \psi_1^\pm \),

\[ \psi_1^\pm (\mathbf{z}, \mathbf{q}) = \chi_1(\mathbf{z}, \mathbf{q}) s_2 s_3. \]

We use here the following notations: \( s_j = s(k_j), r_j = r(k_j) \).

Sector \( K_j^\pm \): \( \psi_R = \psi_3^\pm \),

\[ \psi_3^\pm (\mathbf{z}, \mathbf{q}) = \chi_3(\mathbf{z}, \mathbf{q}) s_1 s_2. \]

Sector \( K_j^\pm \): \( \psi_R = \psi_2^\pm \),

\[ \psi_2^\pm (\mathbf{z}, \mathbf{q}) = \chi_2(\mathbf{z}, \mathbf{q}) s_1 + \chi_2(\mathbf{z}, \tau_3 \mathbf{q}) s_2 r_3. \]

Sector \( K_j^\pm \): \( \psi_R = \psi_1^\pm \),

\[ \psi_1^\pm (\mathbf{z}, \mathbf{q}) = \chi_1(\mathbf{z}, \mathbf{q}) + \chi_1(\mathbf{z}, \tau_2 \mathbf{q}) r_2 s_1 + \chi_1(\mathbf{z}, \tau_3 \mathbf{q}) r_2 r_3 + \chi_1(\mathbf{z}, \tau_1 \mathbf{q}) r_3. \]

Sector \( K_j^\pm \): \( \psi_R = \psi_3^\pm \),

\[ \psi_3^\pm (\mathbf{z}, \mathbf{q}) = \chi_3(\mathbf{z}, \mathbf{q}) + \chi_3(\mathbf{z}, \tau_2 \mathbf{q}) r_2 s_3 + \chi_3(\mathbf{z}, \tau_3 \mathbf{q}) r_2 r_3 + \chi_3(\mathbf{z}, \tau_1 \mathbf{q}) r_1. \]

The total field \( \psi_R \) is defined by the formula

\[ \psi_R = \theta_1^+ \psi_1^+ + \theta_3^- \psi_3^- + \theta_2^+ \psi_2^+ + \theta_3^- \psi_2^- + \theta_1^+ \psi_1^- + \theta_3^+ \psi_3^-. \]

The notation \( \theta_j^{(\pm)} \) is used here for the characteristic function of the corresponding sector \( K_j^\pm \),

\[ \theta_1^+ + \theta_3^- + \theta_2^+ + \theta_3^- + \theta_1^+ + \theta_3^+ = 1. \]

In this formula the value of the field \( \psi_R \) on the boundaries of the sectors is not defined. On all boundary rays except two, directed along the vectors

\[ \mathbf{q}_{23} \equiv \tau_2 \tau_3 \mathbf{q}, \quad \mathbf{q}_{21} \equiv \tau_2 \tau_1 \mathbf{q}, \]

the field is smooth, and its discrepancy is equal to zero everywhere except the two vectors.

To show this we have to consider the explicit expressions for the ray fields near the boundaries of the adjacent sectors and control their coincidence. Consider, for example, the common boundary \( \mathbf{q} \) of two sectors \( K_1^+ \) and \( K_1^- \). For sufficiently large \( \mathbf{z} \) the solutions \( \chi_1 \) and \( \chi_3 \) can be replaced by their elementary simplifications on the subsets where the potentials are
equal to 0. It is not hard to check that both the solutions \( \chi_1(\mathbf{z}, \mathbf{q}) \) and \( \chi_3(\mathbf{z}, \mathbf{q}) \) near \( \mathbf{q} \) are correspondingly equal to

\[
\begin{align*}
\chi_1(\mathbf{z}, \mathbf{q}) & = s(k_1) e^{i\kappa_1 k_1} e^{i\alpha_1 p_1}, \\
\chi_3(\mathbf{z}, \mathbf{q}) & = s(k_3) e^{i\kappa_3 k_1} e^{i\alpha_1 p_1}.
\end{align*}
\]  

(18) (19)

Therefore, the ray solution is continuous on the ray \( \mathbf{q} \). Similar, but, may be, a little bit more complicated computations allow us to control the continuity on all boundaries except two exceptional cases mentioned earlier.

2.5. Diffraction corrections

The diffraction corrections on rays directed along the vectors \( \mathbf{q}_{23} \) and \( \mathbf{q}_{21} \) can be constructed quite easily. We will use for that the known Sommerfeld formulas that describe the diffraction of the plane wave by the edge of the semi-screen. Consider the sector \( \lambda_{231} \) containing \( \mathbf{q}_{23} \). Introduce the polar coordinates \((r, \phi)\). Let us orient the angle from \( \mathbf{I}_2 \) to \( \mathbf{I}_3 \). Let \( \omega_{23} \) corresponds to \( \mathbf{q}_{23} \). Introduce four angles \( 0 < \omega_1 < \omega_2 < \omega_3 < \omega_4 < \pi/3 \). Consider the open covering of the interval \((0, \pi/3)\) by the subintervals \((0, \omega_2), (\omega_1, \omega_4), (\omega_3, \pi/3)\) and introduce a subordinated partition of unit:

\[
1 = \zeta_1 + \zeta_2 + \zeta_3.
\]  

(20)

Further consider the function

\[
\Phi(\alpha) = e^{-i\frac{\pi}{2}} \int_0^\infty e^{i\alpha t} dt.
\]  

(21)

Note that

\[
\Phi(\alpha) \rightarrow 1, \quad \text{as} \ \alpha \rightarrow +\infty, \quad \Phi(\alpha) \rightarrow 0, \quad \text{as} \ \alpha \rightarrow -\infty.
\]  

(22)

In more detail,

\[
\Phi(\alpha) = 1 + e^{-i\frac{\pi}{2}} \frac{e^{i\omega_3}}{2\alpha} + \Delta \Phi(\alpha), \quad \Delta \Phi(\alpha) = - \frac{e^{-i\frac{\pi}{2}}}{\sqrt{\pi}} \int_{\omega_3}^\infty \frac{e^{i\alpha t}}{2\alpha^2} dt = O(\alpha^{-3}),
\]

when \( \alpha \rightarrow +\infty. \)

Introduce the function

\[
\Phi_1^{(23)} = \Phi(\text{sign}(\omega_{23} - \omega)||\mathbf{q}_{23}||\mathbf{z}||\mathbf{q}_{23}|^{1/2}),
\]  

(23)

\[
\Phi_2^{(23)} = \Phi(\text{sign}(\omega - \omega_{23})||\mathbf{q}_{23}||\mathbf{z}||\mathbf{q}_{23}|^{1/2}).
\]  

(24)

It is known that

\[
\Phi = e^{i\mathbf{(x,q_{23})}} \Phi_j^{(23)}
\]  

(25)

satisfies the Helmholtz equation \(-\Delta \Phi - E\Phi = 0. \)

Now we can describe the diffraction corrections to the ray approximation on \( \lambda_{231} \). For that the ray field \( \psi_R = \theta^*_1 \psi_2^* + \theta^*_2 \psi_1 \) in the sector \( \lambda_{231} \) is replaced by

\[
\psi_D^{(23)} = \psi_R + \zeta_3 e^{i\mathbf{q_{23}q_{23}}} \left[ R_1 (\Phi_1^{(23)} - \theta^*_1 \psi_1) + R_2 (\Phi_2^{(23)} - \theta^*_2 \psi_2) \right].
\]  

(26)

\[
R_1 = r_1 s_2 r_3, \quad R_2 = r_3 r_2 s_1 + s_3 r_2 r_1.
\]

Note that the field \( \psi_R \) on the interval \((\omega_1, \omega_4)\) contains the discontinuous component

\[
\psi_j = e^{i\mathbf{q_{23}q_{23}}} \left[ \theta^*_2 \psi_1 + \theta^*_1 \psi_2 \right].
\]  

(27)
so the sense of the modification is nothing else but a simple replacement of this component discontinuous on $q_{23}$ by a smooth solution of the Helmholtz equation that outside of $(\omega_2, \omega_3)$ gradually transfers to the original discontinuous component up to a diverging circle wave with a smooth amplitude. Outside of the interval $(\omega_1, \omega_4)$ the function $\psi_D$ coincides with the original ray approximation $\psi_R$.

It is worthy to make a remark concerning the choice of the angles $\omega_m$, $m = 1, 2, 3, 4$. The field we constructed, obviously, depends on this choice. But the difference between the fields corresponding to the two different choices tends to zero faster than the diverging circle wave.

Analogous constructions can also be considered in the sector $\lambda_{312}$. It is also worthy to introduce here the polar coordinates, and again to suppose that the angle $\omega$ varies in the same limits with the same orientation, from $1_2$ to $-1_2$. We again can introduce the angles $\omega_{21}$, $\omega_j$, $j = 1, 2, 3, 4$, and a cutoff function $\zeta_2$. After that the modified field on $\lambda_{312}$ can be described by the formula

$$
\psi_D^{(21)} = \psi_R + \zeta_2 e^{i[q_{21}]z} \left[ R_2(\Phi_1^{(21)} - \theta_3^+) + R_1(\Phi_2^{(21)} - \theta_3^-) \right].
$$

(28)

Here

$$
\Phi_1^{(21)} = \Phi(\text{sign}(\omega_{21} - \omega))[q_{21}||z| - (q_{21}, z)]^{1/2},
$$

(29)

$$
\Phi_2^{(21)} = \Phi(\text{sign}(\omega - \omega_{21}))[q_{21}||z| - (q_{21}, z)]^{1/2}.
$$

(30)

As a result everywhere on $\Gamma$ outside of some circle $C_{r_1}$ with the center at 0 and the radius $r_1$ there appears a smooth approximate wave field $\psi_0$:

$$
\psi_0 = \psi_R \theta_I + \psi_D^{(23)} \theta_{231} + \psi_D^{(21)} \theta_{312}.
$$

(31)

Here $\theta_{231}$ and $\theta_{312}$ are the characteristic functions of the corresponding $\lambda$-sectors, and $\theta_I$ is the characteristic function of their complement. Again there are no jumps on the boundaries of the $\lambda$-sectors.

Consider a circle with the center at the origin. The radius $r_1$ of this circle is defined by the condition that outside of the circle on the rays directed along the vectors $\sigma q$ the sum of the pair potentials is equal to zero. Under this condition the field $\psi_0$ can be additionally modified with the help of the cutoff function $\zeta(|z|)$ that is equal to 0 for $|z| < r_1$ and to 1 for $|z| > r_2$ where $r_1 < r_2$.

The final expression for the approximate field is now

$$
\psi_1 = \psi_0 \zeta.
$$

(32)

2.6. Discrepancy

We remember that there were two proposed criteria that have to be taken into account when we construct the function $\psi_1$. It is sufficiently clear from the explicit formulas that the second one, (2) the difference $\psi_1 - e^{i|z|q}$ contains asymptotically (in the weak sense) only the diverging circle wave, is fulfilled. So we have to check the first one: (1) the discrepancy

$$
Q[\psi_1](z, q) = -\Delta \psi_1 + (v(x_1) + v(x_2) + v(x_3)) \psi_1 - E \psi_1, \quad E = |q|^2,
$$

(33)

sufficiently quickly vanishes at infinity.

From the previous formulas it follows that outside of certain circle of radius $r_1$ the discrepancy is not equal to zero only on some neighborhoods the rays generated by the vectors $q_{23}$ and $q_{21}$. On these neighborhoods the discrepancy vanishes as $|z|^{-5/2}$. It follows from this that the relative scattering amplitude $g(z, q)$, see (12), must be continuous. Here we give for the discrepancy a formula that can be used for the numerical computations of $\psi$. 

9
Consider now the field $\psi_1$ on the neighborhoods of $q_{23}$ and $q_{21}$. It is not hard to see that the discrepancy of this expression is equal to zero on the sectors where there is a derivative of the function $\xi_2$ equal to zero. It means that the discrepancy $Q[\psi_0]$ can differ from zero only on the subintervals $(\omega_1, \omega_2)$ and $(\omega_3, \omega_4)$. This implies that the discrepancy $Q^{(23)}$ on the sector $\lambda_{231}$ can be naturally represented as the sum

$$Q^{(23)} = Q_1^{(23)} + Q_2^{(23)}.$$  

(34)

Similarly, on the sector $\lambda_{312}$

$$Q^{(21)} = Q_1^{(21)} + Q_2^{(21)}.$$  

(35)

All four terms here can be easily computed. The answers are completely analogous. In particular,

$$Q_1^{(23)} = R_1(-\Delta - E) e^{i(q_{23}, z)} (\Phi_1^{(23)} - 1) \xi'_2$$

$$= R_1 \left[ e^{i(q_{23}, z)} (\Phi_1^{(23)} - 1) - \frac{1}{r^2} \xi''_2 - 2i \frac{1}{r^2} (q_{23}, w) e^{i(q_{23}, z)} \Delta \Phi_1^{(23)} \right].$$  

(36)

(37)

where $w$ is a unit vector orthogonal to $z$ and oriented along the direction of increasing $\omega$.

Finally,

$$Q[\psi_0] = Q_1^{(23)} + Q_2^{(23)} + Q_1^{(21)} + Q_2^{(21)}.$$  

(38)

It is easy to see now that all four components of the discrepancy vanish at infinity like $|z|^{-5/2}$.

The final expression for the discrepancy of $\psi_1$ is given by the formula

$$Q[\psi_1] = Q[\psi_0] - 2 \left[ \frac{\partial}{\partial |z|} \psi_0(z, q) \right] \xi' - \psi_0 \frac{1}{|z|} \frac{\partial}{\partial |z|} \frac{\partial}{\partial |z|} \xi.$$  

(39)

There is no problem with the explicit computation of the derivative $\frac{\partial}{\partial |z|} \psi_0(z, q)$.

3. Numerical computations

3.1. The plan

The goal of the computations was to show that the suggested plan is realistic and can be practically used for the computations of the scattered plane wave and the corresponding amplitude of scattering. Some of the obtained results proved to be unexpected and quite interesting.

The pair-particle potential $v(x)$ and the wave vector $q$ are two parameters of the problem. As for $v(x)$ we choose it in the form

$$v(x) = \begin{cases} 2 e^{i(2|x| - 1)}, & |x| < \frac{1}{3} \\ 0, & \text{otherwise}. \end{cases}$$  

(40)

We took the potential from $C^\infty$ in order to reduce the effects of the boundary points of the supp $v$ but any specific choice is not crucial, we could take an arbitrary even potential (non-necessary continuous) with the compact support.

With this potential we computed numerically the solution $\chi(x, k)$ of the one-dimensional Schrödinger equation (5) on the interval $[-\frac{1}{3}, \frac{1}{3}]$, continued it to the exterior of the interval and found the corresponding transition $s(k)$ and reflection $r(k)$ coefficients.

Further we took $E = 4$. For the vector $q$ we used two choices: (1) $k_1 = 1, p_1 = \sqrt{3}$, (2) $k_1 = p_1 = \sqrt{2}$. We will call the first case symmetric, and the second one non-symmetric. In
the first case the field as a function of $z$ is symmetric with respect to the straight line generated by $q$. It was taken for the control.

The function $\psi_R$ was computed directly with the knowledge of the explicit expressions for $\chi_j$; the Fresnel integral was taken from Gnu scientific library (GSL).

The functions $\psi_0(z, q)$ and $\psi_1(z, q)$ were computed with the help of the explicit formulas for them. The discrepancy $Q$ was also computed with the help of the explicit formulas. The radii $r_1 < r_2$ were taken as $r_1 = 4$, $r_2 = 14.5$. We think that this choice reasonably corresponds to the selected value of $|q|$. For the diffraction corrections (and near the origin) the chosen partition of unity corresponds to the function $\zeta(z) = z^3(10 - 15z + 6z^2)$, $0 < z < 1$, where $z$ is the variable relative to the angle $\omega$.

Then we finally considered the boundary problem (15)–(17). Of course, it was the main part of the numerical program of the work. Note that the problem on the disk with the radiation condition on the boundary is not on the spectrum.

For the computations of $\xi$ we mainly used FreeFem++, which is a user friendly language dedicated for solving partial differential equations with the finite element method. All the necessary steps from mesh creation to solving the linear system can be done within the same program in a manner that is not of a black box type. Since we used the finite element method, we introduced the corresponding weak formulation of the problem: find $\xi \in H^1(\Omega)$ such that

$$\int_\Omega \nabla \xi \cdot \nabla w + (v(x_1) + v(x_2) + v(x_3) - E)\xi w \, dx - \int_{\partial \Omega} i\sqrt{E} \xi w \, dS = -\int_\Omega Q w \, dx \quad \forall \, w \in H^1(\Omega).$$

(41)

The finite element discretization of (41) was then done in a standard fashion using quadratic Lagrange elements on a triangular mesh. The computational domain was divided into sub-domains to have the finite element mesh fit better with the support of the potential $V$ and the constructed function $\chi_0$ and the discrepancy $Q$. A relatively uniform mesh was introduced with lengths of triangle edges between 0.15 and 0.48. With a circular domain of radius 190, the total number of degrees of freedom was 3 million. We used Matlab’s solver for large linear systems.

3.2. The results

The results are represented by figures 2–9.

Figures 2 and 3 represent the $\Re(Q)$ (imaginary part has a similar structure) for the non-symmetric and symmetric cases, respectively. The figures show that the discrepancy is localized near the origin (up to $r = r_2$), and near the four rays where the ray field is connected with the Fresnel integrals. The value of the discrepancy near these rays depends on the specific choice of the cutoff functions.

With known $Q$ we can compute $\xi$. Figure 4 represents the field $\xi$, more precisely $\Re(\xi)$ (imaginary part is similar) again for the non-symmetric case. This is the main computational result; therefore, we represent the similar result for $|\xi|$ (the symmetric case) on a much bigger domain of radius 200, figure 5.

Now we can find the complete field $\psi$. Its real part is represented for the non-symmetric and the symmetric cases in figures 6 and 7, respectively. Both pictures are very interesting. They show, in fact, that the field $\psi$ everywhere on the configuration plane is very close to the ray field, for which we have elementary formulas. There are only almost inconspicuous deviations on some specific directions where the ray field itself changes relatively fast.
A certain problem was with the choice of radius $R$. To get more precise results it would be better to take bigger $R$, but the bigger $R$ means the harder computations. The criterion of the compromise was connected with the integral form of the radiation conditions. These conditions are as follows:

(1) the integral

$$\int_{S_R} ds |\xi(z, q)|^2$$

(42)

over the circle $|z| = R$ must be bounded for large $R$;
Figure 4. The correction to $\psi_1$, real part.

Figure 5. The correction to $\psi_1$, absolute value.

(2) the integral

$$\int_{S_R} ds \left| \left( \frac{\partial}{\partial |z|} - i \sqrt{E} \right) \xi(z, q) \right|^2$$

must decrease as $R^{-2}$.

Note that figure 8 shows that the first integral here is asymptotically approaching a constant at sufficiently large $|z|$, and the second integral is quite small for such $|z|$, but does not decrease for the present computations with $R = 190$.

It, probably, means that such a radius is not completely sufficient for the final computations. We decided at the moment to restrict the radius of the circle to 190.
We also considered the corrected boundary condition where the next term of the asymptotic behavior of $\xi$ was also taken into account:

$$\left( \frac{\partial}{\partial r} - i|q| + \frac{1}{2r} \right) \xi|_{r=R} = 0.$$
Figure 8. The $L^2$ norm on the circle.

Figure 9. The behavior of $|\zeta|$ as a function of the angle at the fixed radius $r = R = 50$.

Nevertheless, the correction did not help to stabilize the calculation in smaller domain, as it could be expected. The reason is that the term $\frac{1}{2R}$ appeared to be very small comparatively with the other terms.
The last figure, figure 9, represents the behavior of $|\xi|$ as a function of the angle at the fixed radius $r = R = 50$. We count the angle from the ray $l_1^+$ in the opposite to clockwise direction.

The jumps of the curve occur on the rays where the ray field $\psi_R$ is transformed to the Fresnel integrals, see also figure 3. It is not hard to see that the amplitude of the jumps on this picture are only few percents (2–4%) of the value of the total field.

Acknowledgments

The authors would like to thank Professor V B Belyaev for the fruitful discussions. The work was partially supported by RFBR grant 08-01-00209.

References

[1] Faddeev L D 1963 Trudy Mat. Inst. Steklov 69 3–122 (in Russian)
Faddeev L D 1965 Israel Program for Scientific Translations (Jerusalem) (in English)

[2] Enss V 1979 Ann. Phys. 119 117–32

[3] Derezhinski J and Gerard C 1997 J. Math. Phys. 38 3925–42

[4] Yafaev D R 1992 Mathematical Scattering Theory. General Theory (Providence, RI: American Mathematical Society) p 431

[5] Buslaev V S and Vakulenko A F 1977 Vestnik LGU 13 22–30

[6] Alt E O, Grabberger P and Sandhas W 1967 Nucl. Phys. B 2 167

[7] Dollard J 1964 J. Math. Phys. 5 729

[8] Buslaev V S and Matveev V B 1970 Theor. Math. Phys. 2 367–76

[9] Peterkop R K 1962 Zh. Eksp. Teor. Fiz 43 616 (in Russian)
Peterkop R K 1962 Sov. Phys.—JETP 14 1377 (Engl. Transl.)

[10] Merkuriev S P 1977 Theor. Math. Phys. 32 680

[11] Alt E O and Mukhamedzhanov A M 1994 Phys. Rev. A 47 2004

[12] Macek J H and Ovchinnikov S Yu 1996 Phys. Rev. A 54 1

[13] Rudge M R H 1968 Rev. Mod. Phys. 40 564

[14] Peterkop R K 1977 Theory of Ionization of Atoms by Electron Impact (Boulder, CO: Colorado Associated University Press)

[15] Faddeev L D and Merkuriev S P 1993 Quantum Scattering Theory for Several Particle Systems (Dordrecht: Kluwer)

[16] Merkuriev S P 1980 Ann. Phys. (NY) 130 395

[17] Alt E O and Mukhamedzhanov A M 1992 JETP Lett. 56 435

[18] Alt E O, Sandhas W and Ziegelmann H 1989 J. Phys. B: At. Mol. Opt. Phys. 22 2265

[19] Alt E O and Mukhamedzhanov A M 1994 Phys. Rev. A 47 2004

[20] Kim Y E and Zubarev A L 1997 Phys. Rev. A 56 521

[21] Alt E O and Mukhamedzhanov A M 1993 Phys. Rev. A 47 2004

[22] Alt E O and Sandhas W 1996 Coulomb Interactions in Nuclear and Atomic Few-Body Collisions ed F S Levin and D Micha (New York: Plenum) p 1

[23] Oryu S, Nishimohara S, Shiki N and Chiba S 2007 Phys. Rev. C 75 021001(R)

[24] Deluva A, Fonseca A C and Sauer P U 2005 Phys. Rev. C 71 054005

[25] Kiessky A, Viviani M and Rosati S 2001 Phys. Rev. C 64 024002

[26] Belyaev V B Levin S B and Yakovlev S L 2004 J. Phys. B: At. Mol. Opt. Phys. 37 1369–80

[27] Suslov V M and Vlahovic B 2004 Phys. Rev. C 69 044003

[28] Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 Science 286 2474
Baertschy M, Rescigno T N and McCurdy C W 2001 Phys. Rev. A 64 022709
Bray I 2002 Phys. Rev. Lett. 89 273201

[29] Buslaev V S and Merkur`ev ev S P 1969 Dokl. Akad. Nauk SSSR 189 269–72 (in Russian)
Buslaev V S and Merkur’ev S P 1969 Sov. Phys. Dokl. 14 1055–7 (Engl. Transl.)

[30] Buslaev V S, Merkuriev S P and Salikov S P 1979 Probl. Mat. Fiz. 9 14–30
[29] Buslaev V S, Merkuriev S P and Salikov S P 1979 Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI) (in Russian) 84 16–22
[30] Buslaev V S and Levin S B 2008 Am. Math. Soc. Transl. 225 55–71
[31] Veselova A M 1978 Theor. Math. Phys. 35 180–91
[32] Yang C N 1967 Phys. Rev. Lett. 19 1312
[33] Lieb E and Liniger W 1963 Phys. Rev. 130 1605
[34] McGuire J B 1964 J. Math. Phys. 5 622
[35] Olshanii M 1998 Phys. Rev. Lett. 81 938
[36] Mehta N P, Esry B D and Green C H 2007 Phys. Rev. A 76 022711
[37] Görlitz A et al 2001 Phys. Rev. Lett. 87 130402
[38] Kinoshita T, Wenger T and Weiss D S 2006 Nature 440 900
[39] Kinoshita T, Wenger T and Weiss D S 2004 Science 305 1125
[40] Esteve J et al 2006 Phys. Rev. Lett. 96 130403