ISSN 1062-8738, Bulletin of the Russian Academy of Sciences: Physics, 2016, Vol. 80, No. 8, pp. 942–946. © Allerton Press, Inc., 2016.
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Potential Splitting Approach to the Three-Body Coulomb Scattering Problem

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Abstract—The potential splitting approach is extended to a three-body Coulomb scattering problem. The distorted incident wave is constructed and the driven Schrödinger equation is derived. The full angular momentum representation is used to reduce the dimensionality of the problem. The phase shifts for e^+–H and e^+–He$^+$ collisions are calculated to illustrate the efficiency of the presented method.

DOI: 10.3103/S1062873816080438

INTRODUCTION

The solution to the quantum three-body problem of Coulomb scattering is difficult due to complex boundary conditions for the wave function in different asymptotic regions. Using the complex scaling of coordinates allows us to avoid the use of exact boundary conditions when solving the scattering problem. This approach was first applied to the scattering of two particles with short-range potential [1]. In [2], the formalism was extended to long-range (but non-Coulomb) potentials. The authors proposed truncating the potential at a certain distance, and then using external complex scaling to bypass the non-analyticity of the truncated potential. This approach, however, cannot be used for Coulomb interactions. It is known that when the truncation radius tends to infinity, the solution to the problem with a truncated Coulomb potential does not tend to the solution of the problem with the full Coulomb potential. In [3–7], the authors proposed a method to avoid this difficulty using the potential splitting approach. Two-body single-channel and multi-channel scattering problems were examined in [3–5], and a three-body problem in the Temkin–Poet approximation in [6, 7]. A three-dimensional distorted incident wave for the split Coulomb potential was constructed in [5].

In this work, we extend the potential splitting approach to the problem of full three-dimensional Coulomb scattering. We construct a distorted incident wave and derive the inhomogeneous Schrödinger equation. A representation of full angular momentum is used to reduce the problem's dimensionality. The phases of scattering for positron collisions with hydrogen and helium positive ions are calculated in order to demonstrate the proposed method.

STATEMENT OF THE PROBLEM

This work deals with the scattering in a system consisting of three non-relativistic charged particles with pair interactions. Jacobi coordinates $\vec{x}_\alpha, \vec{y}_\alpha$ are used to describe the system:

$$\begin{cases} \vec{x}_\alpha = \vec{r}_\beta - \vec{r}_\gamma \\ \vec{y}_\alpha = \vec{r}_\alpha - \dfrac{m_\beta \vec{r}_\beta + m_\gamma \vec{r}_\gamma}{m_\alpha + m_\beta + m_\gamma}, \end{cases} \tag{1}$$

where indices α, β and γ represent the cyclic permutation of numbers $\{1,2,3\}$. Vectors $\vec{r}_\alpha$ and m_α fix the position of particle α and its mass. The wavefunction in the center-of-mass coordinate system obeys the Schrödinger equation

$$\left[-\frac{1}{2\mu_\alpha^x}\Delta_{x_\alpha} - \frac{1}{2\mu_\alpha^y}\Delta_{y_\alpha} + \sum_\beta V_\beta(\vec{x}_\beta)\right] \times \Psi(\vec{x}_\alpha, \vec{y}_\alpha) = E\Psi(\vec{x}_\alpha, \vec{y}_\alpha) \tag{2}$$

with reduced masses $\mu_\alpha^x = m_\beta m_\gamma/(m_\beta + m_\gamma)$, $\mu_\alpha^y = m_\alpha(m_\beta + m_\gamma)/(m_\alpha + m_\beta + m_\gamma)$ and Coulomb potentials $V_\alpha(x_\alpha) = Z_\beta Z_\gamma/x_\alpha$. Before a collision, the initial state of two coupled particles is described by two-body wave function $\varphi_{A_0}(x_\alpha)$. Multi-index $A_0 = \{\alpha;\ n_0, l_0, m_0\}$ includes quantum numbers corresponding to the bound state and the index specifying which two of the three particles form the bound state.

In the asymptotic region $(y_\alpha \to \infty;\ x_\alpha \ll y_\alpha)$, which corresponds to scattering without reconstruction, the wave function has the asymptotics

$$\Psi(\vec{x}_\alpha, \vec{y}_\alpha) \sim \varphi_{A_0}(\vec{x}_\alpha)\Psi_C(\vec{y}_\alpha) + \frac{1}{y_\alpha}\sum_A \varphi_A(\vec{x}_\alpha)F_{AA_0}(\hat{y}_\alpha)\exp[i(p_A y_\alpha - \eta_A \ln(2p_A y_\alpha))]. \quad (3)$$

The first term in (3) describes an incident wave; the second is a superposition of scattered waves. Multi-index A describes different bound states of two particles after a collision; p_A, the momentum of the third particle after collsision; $F_{AA_0}(\hat{y}_\alpha)$, the amplitudes of scattering; and $\eta_A = \mu_\alpha^y Z_\alpha(Z_\beta + Z_\gamma)/p_A$, the Sommerfeld parameter of Coulomb interaction. As a multiplier, the incident wave contains the three-body Coulomb scattering function $\Psi_C(\vec{y}_\alpha)$, expressed explicitly through the degenerate hypergeometric function $M(a,b,c)$:

$$\Psi_C(\vec{y}_\alpha) = \exp[i(\vec{p}_{A_0}, \vec{y}_\alpha) - \pi\eta_{A_0}/2]\Gamma(1 + i\eta_{A_0})M(-i\eta_{A_0}, 1, i(p_{A_0}y_\alpha - (\vec{p}_{A_0}, \vec{y}_\alpha))). \quad (4)$$

In the asymptotic region, $(y_\beta \to \infty; x_\beta \ll y_\beta; \beta \neq \alpha)$, which corresponds to reconstruction, the wave function has the asymptotics

$$\Psi(\vec{x}_\alpha, \vec{y}_\alpha) \sim \frac{1}{y_\beta}\sum_B \varphi_B(\vec{x}_\beta)F_{BA_0}(\hat{y}_\beta)\exp[i(p_B y_\beta - \eta_B \ln(2p_B y_\beta))]. \quad (5)$$

The problem is to determine the scattering amplitudes and calculate such values as the phases of scattering and different scattering cross sections.

POTENTIAL SPLITTING APPROACH

The complex scaling method allows us to solve the problem of scattering using trivial zero boundary conditions for the wave function at infinity. Rotation of radial coordinates of the wave function in the upper halfplane of the complex plane leads to the scattered waves in the asymptotics of the wave function being converted into exponentially decreasing functions that can be made negligibly small by selecting the correct boundary points. Along with the scattered waves, however, there is an incident wave in the asymptotics of the scattered wave function. After complex scaling, this wave diverges exponentially, so a function in the form of the difference between the wave function and the incident wave is studied for correct application of the complex scaling method [1]. This difference satisfies the inhomogeneous Schrödinger equation and is a superposition of the scattered waves in all asymptotic regions. The right side of the inhomogeneous Schrödiger equation is the product of the potential and an incident wave. If the potential is an exponentially decreasing function, then the right side is finite after complex scaling. Direct use of the complex scaling method is in this case possible [2].

The potential is first truncated at a sufficiently great distance, and the external complex scaling is then applied to the equation. The right side of the inhomogeneous Schrödinger equation remains finite after external complex scaling under the condition that the radius of external scaling is larger than that of potential truncation. This approach cannot be used when the potential has a Coulomb tail, since the solution to a problem with a truncated Coulomb potential does not tend to the solution with full Coulomb potential so long as the radius of truncation tends to infinity. It was because of this that the method of potential splitting was developed for Coulomb scattering. A two-body Coulomb problem was studied in [3–5], and a three-body Coulomb problem in the Temkin–Poet approximation in [6, 7].

Let us consider the potential describing the interaction between an incident particle and a bound pair of particles:

$$V^\alpha(\vec{x}_\alpha, \vec{y}_\alpha) = \sum_{\beta\neq\alpha} V_\beta(x_\beta). \quad (6)$$

This potentiial is presented in the form of internal and external components:

$$V^\alpha(\vec{x}_\alpha, \vec{y}_\alpha) = V_R(\vec{x}_\alpha, \vec{y}_\alpha) + V^R(\vec{x}_\alpha, \vec{y}_\alpha), \quad (7)$$

where

$$\begin{cases} V_R = V^\alpha, \ y_\alpha \leq R, \\ V_R = 0, \ y_\alpha > R, \end{cases} \begin{cases} V^R = 0, \ y_\alpha \leq R, \\ V^R = V^\alpha, \ y_\alpha > R. \end{cases} \quad (8)$$

Distorted incident wave $\Psi^R(\vec{x}_\alpha, \vec{y}_\alpha)$ is introduced as a solution to the three-body scattering problem with potential $V_\alpha(x_\alpha) + V^R(\vec{x}_\alpha, \vec{y}_\alpha)$:

$$\left[-\frac{1}{2\mu_\alpha^x}\Delta_{x_\alpha} - \frac{1}{2\mu_\alpha^y}\Delta_{y_\alpha} + V_\alpha(x_\alpha) + V^R(\vec{x}_\alpha, \vec{y}_\alpha)\right]\Psi^R(\vec{x}_\alpha, \vec{y}_\alpha) = E\Psi^R(\vec{x}_\alpha, \vec{y}_\alpha). \quad (9)$$

In analogy with the non-Coulomb case, we study wave function $\Phi(\vec{x}_\alpha, \vec{y}_\alpha) = \Psi(\vec{x}_\alpha, \vec{y}_\alpha) - \Psi^R(\vec{x}_\alpha, \vec{y}_\alpha)$, defined as the difference between the wave function and the distorted incident wave. By definition, this function obeys an inhomogeneous Schrödinger equation whose right side is restricted in y_α:

$$\left[-\frac{1}{2\mu_\alpha^x}\Delta_{x_\alpha} - \frac{1}{2\mu_\alpha^y}\Delta_{y_\alpha} + \sum_\beta V_\beta(x_\beta) - E\right]\Phi(\vec{x}_\alpha, \vec{y}_\alpha) = -V_R(\vec{x}_\alpha, \vec{y}_\alpha)\Psi^R(\vec{x}_\alpha, \vec{y}_\alpha). \quad (10)$$

Since function $\Phi(\vec{x}_\alpha, \vec{y}_\alpha)$ is the difference between the solutions to the two scattering problems, the asymptotics of incident waves compensate for one another, and only scattered waves are found in the result. Equation (10) is thus suitable for use in external complex scaling and numerical solutions. As a first approximation to function $\Psi^R(\vec{x}_\alpha, \vec{y}_\alpha)$, we can use function $\Psi_0^R(\vec{x}_\alpha, \vec{y}_\alpha)$, which is the solution to (9) if external potential $V^R(\vec{x}_\alpha, \vec{y}_\alpha)$ in it is replaced with the corresponding asymptotic expression when $y_\alpha \to \infty$:

$$\left[-\frac{1}{2\mu_\alpha^x}\Delta_{x_\alpha} - \frac{1}{2\mu_\alpha^y}\Delta_{y_\alpha} + V_\alpha(x_\alpha) + \frac{Z_\alpha(Z_\beta + Z_\gamma)}{y_\alpha}\right]\Psi_0^R(\vec{x}_\alpha, \vec{y}_\alpha) = E\Psi_0^R(\vec{x}_\alpha, \vec{y}_\alpha). \quad (11)$$

In this equation, the variables are separated and the solution is presented in the form of the product $\Psi_0^R \times (\vec{x}_\alpha, \vec{y}_\alpha) = \varphi_{A_0}(\vec{x}_\alpha) \times \Psi_C^R(\vec{y}_\alpha)$, in which function $\Psi_C^R(\vec{y}_\alpha)$ determined in [5] is used.

FULL ANGULAR MOMENTUM REPRESENTATION

The wave function is written in the form of an infinite series:

$$\Phi(\vec{x}_\alpha, \vec{y}_\alpha) = \sum_{\tau=\pm 1}\sum_{J=(1-\tau)/2}^{\infty}\sum_{M,M'=-J}^{J} W_{M,M'}^{J,\tau}(\Omega_\alpha)\phi_{M,M'}^{J,\tau}(x_\alpha, y_\alpha, \theta_\alpha), \quad (12)$$

where Ω_α is the set of Euler angles describing rotation from the lab coordinate system to a system rigidly associated with three particles. The rotating coordinate system is chosen such that the new OZ axis is directed along vector $\vec{y}_\alpha$, and vector $\vec{x}_\alpha$ lies in the plane formed by the new OX and OZ axes. Basis functions $W_{M,M'}^{J,\tau}(\Omega_\alpha)$ describe the states with determined angular momentum J and parity τ. They are explicitly expressed through Vigner's D-functions:

$$W_{M,M'}^{J,\tau}(\Omega_\alpha) = \frac{D_{M,M'}^J(\Omega_\alpha) + \tau(-1)^{M'} D_{M,M'}^J(\Omega_\alpha)}{\sqrt{2 + 2\delta_{M,0}}}. \quad (13)$$

Each function $\phi_{M,M'}^{J,\tau} \times (x_\alpha, y_\alpha, \theta_\alpha)$ satisfies the second-order finite system of differential equations in partial derivatives [8]. With zero angular momentum, this system is reduced to a single inhomogeneous equation:

$$\left[-\frac{1}{2\mu_\alpha^x}\frac{\partial^2}{\partial x_\alpha^2} - \frac{1}{2\mu_\alpha^y}\frac{\partial^2}{\partial y_\alpha^2} - \left\{\frac{1}{2\mu_\alpha^x x_\alpha^2} + \frac{1}{2\mu_\alpha^y y_\alpha^2}\right\}\left(\frac{\partial^2}{\partial\theta_\alpha^2} + \mathrm{ctg}\theta_\alpha\frac{\partial}{\partial\theta_\alpha}\right) + \sum_\beta V_\beta(x_\beta) - E\right]$$
$$\times\, \phi_{0,0}^{0,+1} = -\frac{a_0^R}{2\sqrt{\pi}p_{A_0}} V_R(x_\alpha, y_\alpha, \theta_\alpha)\varphi_{A_0}(x_\alpha)\sin(p_{A_0}y_\alpha). \quad (14)$$

In order to simplify the right part of the equation, we assume that the target is in a state with zero angular momentum before a collision. Coefficient a_0^R was calculated in [3]. The asymptotics of function $\phi_{0,0}^{0,+1} \times (x_\alpha, y_\alpha, \theta_\alpha)$ in the channel without reconstruction has the form

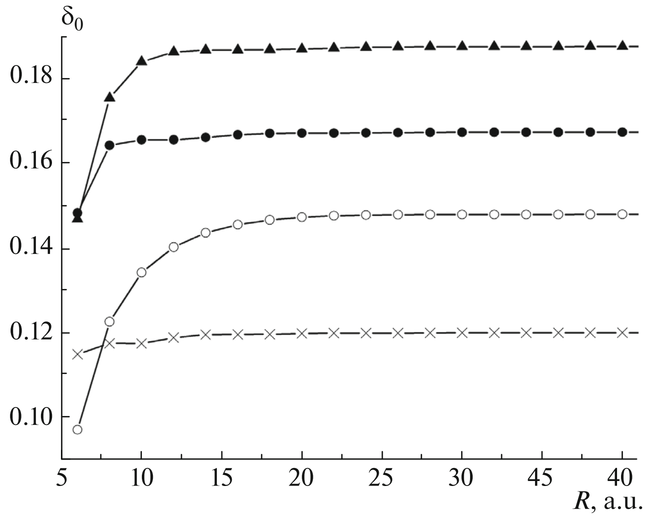

Fig. 1. Phases of elastic scattering with zero total angular momentum as functions of splitting radius R for $e^+{-}He^+$ collisions. Our results correspond to the following momenta of incident positrons: $p_{A_0} = 0.1$ a. u. (white dots); $p_{A_0} = 0.2$ a. u. (triangles); $p_{A_0} = 0.3$ a. u. (black dots); and $p_{A_0} = 0.4$ a. u. (crosses).

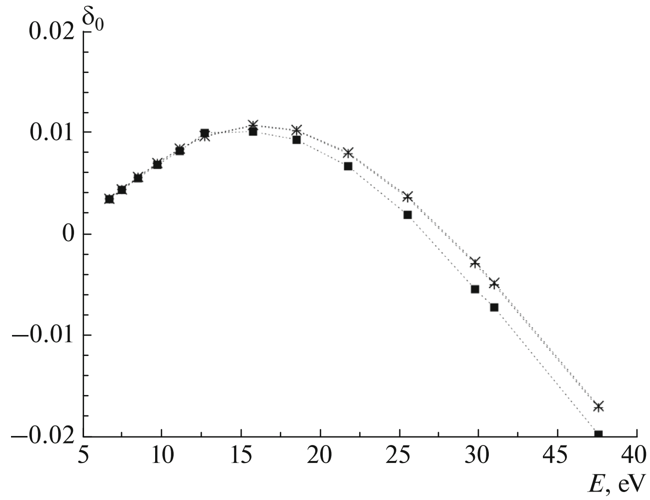

Fig. 2. Phases of elastic scattering with zero total angular momentum as functions of the energy of incident positrons for $e^+{-}He^+$ collisions. The calculation results (diagonal crosses) are compared to the results of [16] (squares) and [17] (upright crosses).

$$\varphi_{0,0}^{0,+1}(x_\alpha, y_\alpha, \theta_\alpha) \sim \frac{1}{y_\alpha}\sum_A \varphi_A(x_\alpha)\exp[i(p_A y_\alpha - \eta_\alpha \log(2p_A y_\alpha))]Y_{l,0}(\theta_\alpha, 0)\tilde{F}_A, \quad (15)$$

where $Y_{l,0}$ are spherical harmonics and $\tilde{F}_A$ represents the constant coefficients. The amplitudes of the transition to different excited states are calculated by the formula

$$F_A = \tilde{F}_A + F_0^R, \quad (16)$$

where F_0^R represents the constants that depend on R, as determined in [3]. Phase δ_0 of scattering with zero total angular momentum is calculated from the amplitude using the formula

$$F_A = e^{2i\sigma_0}\frac{e^{2i\delta_0} - 1}{2ip_A} \quad (17)$$

with Coulomb phase σ_0.The cross section of target excitation at $J = 0$ is calculated using the formula

$$\sigma_A = 4\pi\frac{p_A}{p_{A_0}}|F_A|^2. \quad (18)$$

RESULTS AND DISCUSSION

Using the above method, we calculated the phases of elastic scattering with zero full angular momentum for $e^+{-}H$ and $e^+{-}He^+$ collisions. The numerical approach is based on the finite difference method. A similar approach was used in [9, 10] to calculate the positions of resonances in three-body systems via the complex scaling method. The scattering problem is reduced to solving the system of linear algebraic equations.

The scattering of positrons on hydrogen atoms has now been thoroughly studied, and the literature [11–15] on this subject is fairly extensive. This problem may therefore be seen as a test to verify the method. In addition, many other formulas are simplified, since there is no asymptotic Coulomb interaction between positrons and hydrogen. Figure 1 shows the convergence of the s-wave scattering phase of positrons on hydrogen atoms as radius R grows for different values of incident positron momentum p_{A_0}. Convergence is faster for higher values of the momentum. The values to which the phases converge in the depicted energy range are in fair agreement with the results of other authors. With positron scattering on helium ions, there is asymptotic Coulomb interaction between the incident particle and the target. A number of works have been devoted to this problem [16–20]. Figure 2 shows the dependence of the s-wave scattering phase depending on the energy, compared to the results of [16] and [17]. As can be seen, the agreement with the results from other calculations is very good.

The potential splitting approach thus allows us to perform accurate calculations of partial amplitudes and phases for a three-body Coulomb scattering problem without resorting to additional unjustified approximations.

ACKNOWLEDGMENTS

This work was supported by the Russian Foundation for Basic Research, project no. 14-02-00326; and by St. Petersburg State University as part of project no. 11.38.241.2015. Our numerical calculations were performed using equipment at the St. Petersburg State University Computing Center.

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Translated by G. Dedkov