

Resonances in an *S*-Wave Model of Electron Scattering off Hydrogen-Like Ions

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Abstract—Irregularities in the cross section of electron scattering off hydrogen and hydrogen-like He^+ , Li^{++} , and Be^{+++} ions are studied using an *s*-wave model. The resonance structure and irregularities in the scattering data are compared. A unified approach based on an exterior complex scaling method is used in performing calculations. The potential splitting approach is used for calculations of scattering in systems with asymptotic Coulomb interactions.

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INTRODUCTION

Accurately solving the quantum scattering problem for systems of several particles with Coulomb interaction is of great importance in different fields of modern physics (nuclear, atomic and molecular). This is, however, a very difficult task from both a theoretical and a computational point of view, due to the complex asymptotic behavior of a wave function in coordinate space [1]. There is thus growing interest in methods in which the scattering problem can be solved via the Schrödinger equation with the simplest boundary conditions. One approach that meets this criterion is the complex scaling method in [2–4].

Analysis of theoretical and experimental scattering cross sections often indicates there are a number of irregularities in their behavior, e.g., peaks, dips and jumps. These irregularities are usually associated with resonance states being in the system, i.e., states with finite lifetimes. The Breit–Wigner formalism is often applied to describe the behavior of scattering data in the vicinity of resonance [5]. However, it can be used only in the neighborhood of narrow isolated resonances. Generally, the contributions from different resonant states can overlap and significantly alter the behavior of a scattering cross section. The effect of wide resonances can be hard to identify but cannot be ignored. The most complete picture of scattering can thus be built when there is a calculated scattering cross section and the positions and widths of the resonances are obtained independently. The complex scaling method provides a mathematically correct way of calculating the resonances of a system [6].

In this work, we present a joint description of scattering processes and resonances in an *s*-wave model of electron scattering off hydrogen and hydrogen-like He^+ , Li^{++} , and Be^{+++} ions. A corresponding model for

hydrogen was proposed by Temkin [7] and Poet [8] and is known as the Temkin–Poet (TP) model. It can naturally be generalized to one-electron ions. Though the TP model represents a simplified approach to the problem of three-particle scattering, it retains many key features of the original task. This model is often used to test different approaches to solving the scattering problem, allowing us to use relatively moderate resources as compared to the full task computation.

A unified approach based on the method of exterior complex scaling is used in calculating resonances and the processes of scattering. The unified approach allows us to minimize calculation errors and makes it much easier to compare results. A newly developed method of potential splitting is used to solve the problem of scattering with Coulomb interaction [9, 10].

POTENTIAL SPLITTING METHOD IN THE TP MODEL

The Hamiltonian of the TP model for ions is written in the form

$$H = -\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} - \frac{Z}{r_1} - \frac{Z}{r_2} + V_{12}(r_1, r_2), \quad (1)$$

where r_i is the distance between the nucleus and the i -th electron; Z is the charge of nucleus; and the electron–electron potential in the *s*-state is $V_{12}(r_1, r_2) = 1/\max(r_1, r_2)$. Wave function Ψ of the system satisfies the Schrödinger equation with Hamiltonian (1). Due to the identity of electrons, the wave function must be symmetrized with respect to the permutation of electrons. Symmetrized wave function Ψ^S is given by

$$\Psi^S(r_1, r_2) = \frac{1}{\sqrt{2}} \left(1 + (-1)^S P_{12} \right) \Psi(r_1, r_2), \quad (2)$$

where states with spin $S = 0, 1$ correspond to the singlet and triplet states, respectively. Permutation operator P_{12} swaps the places of coordinates r_1 and r_2 . Since the permutation operator commutes with Hamiltonian (1), the symmetrized wave function satisfies the same Schrödinger equation as the wave function Ψ .

Let us briefly describe the potential splitting method in the TP model [10]. We introduce indicator χ^R of domain $r \geq R$,

$$\chi^R(r) = \begin{cases} 0, & r < R \\ 1, & r \geq R \end{cases}, \quad (3)$$

and its complement $\chi_R = 1 - \chi^R$. The potential is defined by

$$V^R = -\frac{Z}{r_2} - \left(\frac{Z}{r_1} + V_{12}(r_1, r_2) \right) \chi^R(r_1). \quad (4)$$

Asymptotic Hamiltonian H^R is fixed in the terms of potential

$$H^R = -\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} + V^R. \quad (5)$$

$$\left(-\frac{1}{2} \frac{\partial^2}{\partial r_1^2} - \frac{1}{2} \frac{\partial^2}{\partial r_2^2} - \frac{Z}{r_1} - \frac{Z}{r_2} + V_{12}(r_1, r_2) - E \right) \Phi^S(r_1, r_2) = -\frac{1}{\sqrt{2}} (1 + (-1)^S P_{12}) \left(-\frac{Z}{r_1} + V_{12} \right) \chi_R(r_1) \Psi^R(r_1, r_2). \quad (9)$$

Since the right-hand side of this equation is non-analytical when $r_i = R$, we can only use the method of exterior complex scaling with radius $Q \geq R$. Exterior complex scaling can be used, since the solution to (9) and the right side of this equation remain finite upon turning the coordinates in the upper complex half-plane. After applying complex scaling to Eq. (9), the solution to the transformed equation is diminished rapidly at great distances, so the equation can be solved with zero boundary conditions at infinity; this

The role of an incident wave in the potential splitting approach is played by solution Ψ^R to Schrödinger equation $H^R \Psi^R = E \Psi^R$. This solution can be written in explicit form

$$\Psi^R(r_1, r_2) = \Psi_c^R(r_1, k_i) \varphi_i(r_2), \quad (6)$$

where $\varphi_i(r_2)$ is the function of the bound state of a two-particle system with energy ε_i . Momentum k_i of an incident particle is related to total energy E of the system: $E = \varepsilon_i + k_i^2/2$. Function Ψ_c^R satisfies the equation

$$\left(-\frac{1}{2} \frac{d^2}{dr_1^2} - \frac{(Z-1)\chi^R(r_1)}{r_1} - k_i^2 \right) \Psi_c^R(r_1, k_i) = 0. \quad (7)$$

Its explicit expression can be found in [10].

Using this representation for an incident wave, we can rewrite the Schrödinger equation for function Ψ^S in inhomogeneous form. By writing the entire wave function in the form

$$\Psi^S = \Phi^S + \frac{1}{\sqrt{2}} (1 + (-1)^S P_{12}) \Psi^R, \quad (8)$$

we obtain the following inhomogeneous equation for Φ^S :

greatly simplifies formulation of the boundary value problem. In the region not subjected to complex scaling, $r_i \leq Q$, the solution to the transformed equation coincides with the that of original one, allowing us to obtain the correct solution at fairly great R .

Having obtained the solution to (9), we can use the familiar asymptotics in [1] by projecting the solution onto the pair state in an output channel. Singling out the asymptotic behavior of the wave function, we find the amplitude of scattering from channel i into channel j :

$$f_{ji}^S(k_j) = \lim_{r_1 \rightarrow \infty} \sqrt{2} (U_0(\eta_j, k_j r_1))^{-1} \int_0^R dr_2 \varphi_j(r_2) \Phi^S(r_1, r_2). \quad (10)$$

In the latter equation, an outgoing Coulomb wave $U_0(\eta_j, k_j r_1)$ is defined in the terms of regular F_0 and irregular G_0 Coulomb functions

$$U_0(\eta_j, k_j r_1) = e^{-i\sigma_0} [G_0(\eta_j, k_j r_1) + iF_0(\eta_j, k_j r_1)],$$

where $\eta_j = -(Z-1)/k_j$ is the Sommerfeld parameter. The scattering cross sections are expressed through the amplitudes in the standard way:

$$\sigma_{ji}^S(k_j) = 4\pi \frac{k_j}{k_i} \left| f_{ji}^S(k_j) \right|^2.$$

RESULTS AND DISCUSSION

The finite element method in [10], used earlier for calculating resonances in three-body systems [11], was employed to find the numerical solution to Eq. (9).

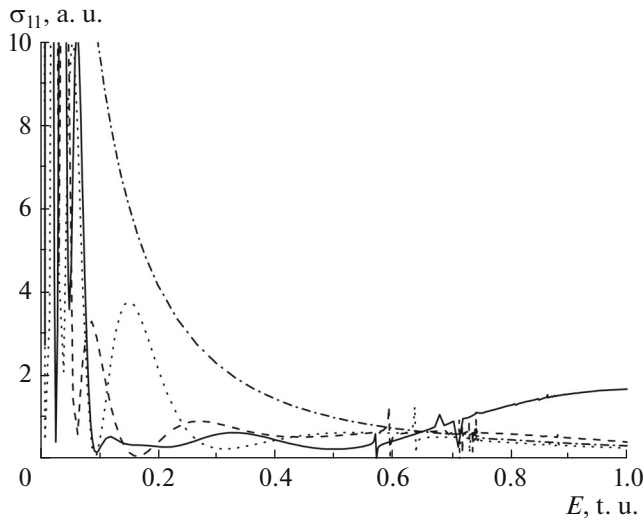


Fig. 1. Normalized singlet scattering cross section as a function of energy in channel $1s \rightarrow 1s$ for the scattering of electrons on hydrogen atoms (dashed-and-dotted line), helium ions (dotted line), lithium ions (dashed line), and beryllium ions (solid line).

The parameters of the numerical scheme were chosen so that the error did not affect the results within the specified accuracy. The radius of complex scaling was chosen equal to that of potential splitting, $Q = R$, and was 91 a.e. for all of the investigated systems.

The calculation results for different systems are easily compared using specially chosen units of energy: threshold units (t. u.) [12, 13]. These units depend on the investigated system and are determined in terms of atomic units (a. u.):

$$1 \text{ t. u.} = \frac{Z^2}{2} \text{ a. u.} \quad (11)$$

The bonding energy was therefore the same for all of the investigated systems: 1 t. u. These units are used below unless otherwise specified.

Figure 1 shows the computed cross sections of singlet scattering in channel $1s \rightarrow 1s$ for hydrogen atoms and He^+ , Li^{++} , and Be^{+++} ions. The energy of scattering is counted from the ground state, and the values of the cross sections are multiplied by Z^2 for easy comparison of different systems. There is a considerable difference between scattering on hydrogen and on ions: there are no oscillations or resonance peaks in the scattering cross section for hydrogen at low energies. These differences are due to the lack of asymptotic Coulomb interaction with hydrogen atoms. The behavior of the scattering cross sections of ions has common features: a single resonance in the vicinity of 0.6 t. u. and an endless series of resonances accumulated close to (below) the two-body threshold with an energy of 0.75 t. u. Such series also exist near subse-

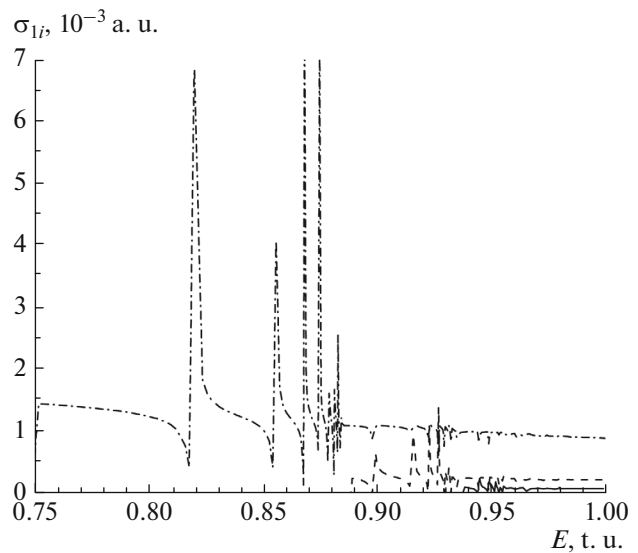


Fig. 2. Singlet scattering cross section as a function of energy in channels $1s \rightarrow 2s$ (dashed-and-dotted line), $1s \rightarrow 3s$ (dotted line), and $1s \rightarrow 4s$ (solid line) for the scattering of electrons on lithium ions.

quent thresholds, but they are virtually indistinguishable in the channel $1s \rightarrow 1s$.

In order to examine the near-threshold behavior of scattering cross sections in more detail, let us consider the transition cross sections $1s \rightarrow 2s$, $1s \rightarrow 3s$, and $1s \rightarrow 4s$ for Li^{++} shown in Fig. 2. We can clearly see the series of resonances converging to thresholds with energies of 0.88(8), 0.9375, and 0.96 t. u. Since the distance between thresholds shrinks as the number grows, the resonances become narrower and their accurate imaging becomes difficult. It is also important that there are irregularities at the same energy in any open scattering channel, but the amplitudes of peaks in different channels can differ significantly. This is in good agreement with the Breit–Wigner multichannel formula for the elements of a scattering matrix [14]:

$$S_{ij}(E) = \exp(2i\gamma_i)\delta_{ij} - i \exp(i(\gamma_i + \gamma_j)) \frac{\sqrt{\Gamma_i \Gamma_j}}{E - E_R} \quad (12)$$

Here, γ_i is the background phase; E_R is the complex energy of resonance; and Γ_i is the partial resonance width, which is not accurately defined as it is difficult to calculate [15].

Determining the positions and especially the widths of the resonances of scattering cross sections shown in Figs. 1 and 2 can be quite challenging, particularly in the ranges of energy where there are many resonances and they are narrow. In addition, the calculations may need a very small energy step in order not to miss possible features in the cross sections. In this situation, preliminary determination of the positions and widths of resonances can help to identify

Complex energy values of several resonances for helium ions ($Z = 2$), lithium ions ($Z = 3$) and berillium ions ($Z = 4$). The energy is counted from the ionization threshold. The numbers in parentheses specify the decimal degree

$Z = 2$	$Z = 3$	$Z = 4$
$-0.3614 - i 6.00 (-4)$	$-0.4049 - i 3.61 (-4)$	$-0.4276 - i 2.31 (-4)$
$-0.2924 - i 4.52 (-7)$	$-0.3134 - i 3.81 (-7)$	$-0.3247 - i 2.79 (-7)$
$-0.2860 - i 1.42 (-4)$	$-0.3071 - i 1.22 (-4)$	$-0.3192 - i 8.86 (-5)$
$-0.2710 - i 2.11 (-7)$	$-0.2831 - i 2.07 (-7)$	$-0.2898 - i 1.63 (-7)$
$-0.2688 - i 5.83 (-5)$	$-0.2810 - i 5.13 (-5)$	$-0.2880 - i 3.71 (-5)$
$-0.1608 - i 6.43 (-4)$	$-0.1801 - i 3.86 (-4)$	$-0.1902 - i 2.44 (-4)$
$-0.1361 - i 3.50 (-6)$	$-0.1477 - i 2.71 (-6)$	$-0.1539 - i 1.91 (-6)$
$-0.1326 - i 2.16 (-4)$	$-0.1444 - i 1.74 (-4)$	$-0.1511 - i 1.22 (-4)$

potentially interesting ranges of energy. The table shows the energies of the deepest resonances in the series converging to the second (-0.25 t. u.) and third ($-1/9$ t. u.) thresholds. Except at the deepest level, they form pairs with close values of the real parts of energy and very different widths. These pairs of resonances, like the pairs of bound states, correspond to the singlet and triplet states of the system. The triplet states are narrower by several orders of magnitude, corresponding to the almost complete lack of visible resonance effects in the triplet scattering cross section. This effect is entirely consistent with Breit–Wigner formula (12).

CONCLUSIONS

We studied features in the scattering cross sections of electrons on hydrogen and hydrogen-like He^+ , Li^{++} , and Be^{+++} ions using an s -wave model, and compared them to resonances in the corresponding triplet systems. The s -wave model is a simplified two-dimensional variant of the three-body problem that retains many important features of the full three-dimensional three-body problem. A common approach based on the method of external complex scaling is used to calculate scattering processes and resonances. This approach allows us to minimize calculation errors and make a much more reliable comparison of the calculated scattering data and resonance states. The potential splitting method was used to solve the scattering problem with asymptotic Coulomb interaction.

It should be noted that any comparison of the resonance structure in scattering cross sections and the actual resonances of a system should include not only an analysis of the resonance energies themselves, but also one of the effect resonance levels have on the scattering cross sections, as was done in [16] for two-body systems. Generalization of the technique used there would seem to be quite simple, but this has yet to be done for three-body systems.

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REFERENCES

1. Merkur'ev, S.P. and Faddeev, L.D., *Kvantovaya teoriya rasseyaniya dlya sistem neskol'kikh chastits* (Quantum Scattering Theory for Several-Particle Systems), Moscow: Nauka, 1985.
2. Nuttall, J. and Cohen, H.L., *Phys. Rev.*, 1969, vol. 188, p. 1542.
3. Rescigno, T.N., Baertschy, M., et al., *Phys. Rev. A*, 1997, vol. 55, p. 4253.
4. Volkov, M.V., Elander, N., et al., *Europhys. Lett.*, 2009, vol. 85, p. 30001.
5. Breit, G. and Wigner, E., *Phys. Rev.*, 1936, vol. 49, p. 519.
6. Balslev, E. and Combes, J.M., *Commun Math. Phys.*, 1971, vol. 22, p. 280.
7. Temkin, A., *Phys. Rev.*, 1962, vol. 126, p. 130.
8. Poet, R., *J. Phys. B*, 1978, vol. 11, p. 3081.
9. Elander, N., Volkov, M., et al., *Few-Body Syst.*, 2009, vol. 45, p. 197.
10. Yarevsky, E., Yakovlev, S.L., et al., *J. Phys. B: At. Mol. Opt. Phys.*, 2015, vol. 48, p. 115002.
11. Elander, N. and Yarevsky, E., *Phys. Rev. A*, 1998, vol. 57, p. 3119.
12. Bray, I. and Clare, B., *Phys. Rev. A*, 1997, vol. 56, p. R1694.
13. Bartschat, K. and Bray, I., *Phys. Rev. A*, 1997, vol. 55, p. 3236.
14. Taylor, J.R., *Scattering Theory: the Quantum Theory of Nonrelativistic Collisions*, Dover, 2006.
15. Peskin, U., Moiseyev, N., and Lefebvre, R., *J. Chem. Phys.*, 1990, vol. 92, p. 2902.
16. Shilyaeva, K., Elander, N., and Yarevsky, E., *J. Phys. B: At. Mol. Opt. Phys.*, 2009, vol. 42, p. 044011.

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