On the scattering of the electron off the hydrogen atom and helium ion below and above the ionization threshold: Temkin-Poet model

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The importance of scattering problem for quantum systems of charged particles can hardly be overestimated. A key problem here is a complicated asymptotic behavior of the wave function in coordinate space. Thus interest in methods that would reduce the scattering problem to a problem with simplified in some sense boundary conditions is always high.

One of such approaches is based on the method of complex rotations. Originally, this approach was based on the uniform rotations and could only be applied to problems involving finite range or exponentially decreasing potentials. It was modified in [1] in such a way that longer range potentials could be studied. The potential $V(r)$ was replaced by a finite cut potential $V_R(r)$, $V_R(r) = 0$ for $r \geq R$. As $V_R(r)$ is not analytic, the external complex rotation method has to be employed.

The approach [1] is inapplicable to the Coulomb scattering problem since the cutoff of the Coulomb potential at any R distorts the asymptotic behavior of the solution at infinity. In [2,3], we have shown how the method of external complex rotations can be applied to systems involving Coulomb interaction. Instead of cutting off the potential at a point R, we represent it as the sum $V(r) \equiv V_R(r) + V^R(r)$. Then the scattering problem is solved for the potential tail $V^R(r)$, and this solution is used as an incident wave Ψ^R. Subtracting Ψ^R from the total wave function, we obtain a function whose asymptotic behavior is that of a diverging wave. Applying the external complex rotation to the non-homogeneous Schrödinger equation, we arrive at the boundary-value problem with zero boundary conditions.

Here, we apply this idea to the Temkin-Poet (TP) model of the electron scattering on the hydrogen atom [4] ($Z = 1$) and on the positive Helium ion [5] ($Z = 2$). The TP model is a S-wave model of three-body scattering, featuring nonetheless most of essential properties and difficulties of the original scattering problem. We recast the Schrödinger equation in the electron coordinates r_1, r_2 in the driven form in such a way that the total wave function Ψ is represented in the form $\Psi = \Psi^R + \Phi$. The incoming wave Ψ^R satisfies the Schrödinger equation with the tail Coulomb potential and the function Φ satisfies

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial r_1^2} - \frac{1}{2}\frac{\partial^2}{\partial r_2^2} - \frac{Z}{r_1} - \frac{Z}{r_2} + V_{12}(r_1, r_2) - E\right]\Phi(r_1, r_2) =$$
$$-\frac{1}{\sqrt{2}}(1 + (-1)^S P_{12})\left(-\frac{Z}{r_1} + V_{12}(r_1, r_2)\right)\chi^R(r_1) a_R \hat{j}_0(k_i r_1)\varphi_i(r_2), \qquad (1)$$

where $S = 0, 1$ for the singlet or triplet scattering, respectively. The electron-electron interaction in this model is given by $V_{12}(r_1, r_2) = 1/\max\{r_1, r_2\}$. The function χ^R is defined as $\chi^R(r_1) = 1$ for $r_1 < R$, and $\chi^R(r_1) = 0$ for $r_1 \geq R$. The operator P_{12} interchanges the coordinates r_1 and r_2. The value of a_R follows from the matching conditions at $r_1 = R$.

The r.h.s. of Eq. (1) decreases in both coordinates, so this equation can be solved with the exterior complex scaling method. We find the wave function $\Psi(r_1, r_2)$ in the region $r_1, r_2 \leq R$, and then find amplitudes and cross sections corresponding to various scattering processes in the system. Both elastic and ionization amplitudes can be determined.

For the TP model of the electron-hydrogen scattering, accurate benchmark results are available [6]. We compare our data with the results of paper [6] in order to demonstrate the accuracy of our numerical approach which is based on the finite element method. We have also investigated its convergence properties.

The electron-He^+ calculations in the frame of the TP model [5] are rather scarce. For this system, Eq. (1) differs from a naive equation derived without taking into account special properties of the Coulomb potential. This naive equation can be derived by putting $a_R = 1$ in Eq. (1). The factor $|a_R|^2$ is explicitly present in all expressions for the cross sections so it makes a difference between the correct and naive results. As one could expect, this factor is relatively small for high energies but grows for lower energies.

With the approach developed, we have performed calculations of the excitation as well as ionization cross-sections for the electron-He^+ scattering. As an example, we plot on Fig. 1 the $1S$-$2S$ excitation cross-section as a function of the electron energy. We have found that

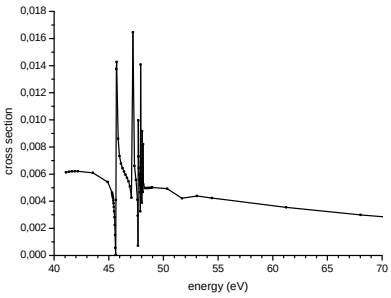

Figure 1: Singlet (spin weight included) $1S$-$2S$ excitation cross-section results for the TP model of e-He^+ scattering as a function of the incident electron energy.

our approach demonstrates good stability and high accuracy for the scattering problem. In contrast to the close-coupling and R-matrix approaches [5], our calculations do not suffer from artificial noise and oscillations.

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