Two-body Coulomb scattering and complex scaling

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Two-body Coulomb scattering and complex scaling

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Abstract. The two-body Coulomb scattering problem is studied with the complex scaling method. Our splitting method [1], on partial wave level, simplifies the scattering boundary condition. The scattered part of the wave function is square integrable. This property makes the numerical solution easier.

1. Introduction

The method of complex scaling (CS) has been successfully applied in many areas of quantum physics, but for scattering problems the CS procedure can only be applied to short-range potentials, which limits the applicability of CS in atomic and nuclear physics.

It has been shown in the Ref. [2] that scattering calculations with the exterior CS can be successfully performed for long-range interactions as well. Nevertheless, the exterior CS method has been under scrutiny since an artificial cutoff of some of the interaction may cause troubles. Recently, however, it has been shown [3] that the standard CS can be applied to scattering problems even in the presence of the pure Coulomb interaction. The method is based on the two-potential formalism. An alternative technique is presented below.

The full scattering solution is written in the form

$$\psi^{+}(\mathbf{k},\mathbf{r}) = \phi_0(\mathbf{k},\mathbf{r}) + \psi^{sc+}(\mathbf{k},\mathbf{r}), \tag{1}$$

where $\psi^{sc+}(\mathbf{k},\mathbf{r})$ is the scattered wave, and $\phi_0(\mathbf{k},\mathbf{r})$ is a known function. From the Schrödinger equation the so called driven Schrödinger equation can be derived for the scattered wave:

$$(E - \hat{H})\psi^{sc+}(\mathbf{k},\mathbf{r}) = S(\mathbf{k},\mathbf{r}), \tag{2}$$

where the source term is given by $S(\mathbf{k},\mathbf{r}) = (\hat{H} - E)\phi_0(\mathbf{k},\mathbf{r})$.

2. Theory

We have found that the choice of the so called Coulomb-modified plane wave (CMPW),

$$\phi_0(\mathbf{k},\mathbf{r}) = e^{i\mathbf{kr}}(kr - \mathbf{kr})^{i\gamma}, \tag{3}$$

does not simplify the boundary condition from the point of view of the complex scaling.

We rather split the wave function into incoming and scattered waves at the partial-wave level. The exact incoming wave is $\psi_{i,l}(k,r)$ [4] and we write

$$\psi_l^{+}(k,r) = \psi_{i,l}(k,r) + \psi_l^{sc+}(k,r), \tag{4}$$

where

$$\psi_{i,l}(k,r) = \omega_{i,l}(k,r) + \chi_l(k,r) \tag{5}$$

and

$$\omega_{i,l}(k,r) = e^{-ikr}e^{\gamma\pi/2}(-1)^{l+1}(2ikr)^l U(l+1-i\gamma, 2l+2, 2ikr), \tag{6}$$

$$\chi_l(k,r) = \frac{e^{ikr+\gamma\pi/2}}{2ikr}\frac{(-1)^l}{(2ikr)^l}\frac{\Gamma(2l+1)}{\Gamma(l+1-i\gamma)}\sum_{n=0}^{l}\frac{(-1)^n(i\gamma-l)_n}{(-2l)_n n!}(2ikr)^n, \tag{7}$$

with U being the confluent hypergeometric function. For the driven radial Schrödinger equation direct calculation gives the following source term

$$S_l(k,r) = \frac{e^{ikr+\gamma\pi/2}}{2r^2\Gamma(-i\gamma)}. \tag{8}$$

After CS by scaling angle θ, which satisfies the condition $0 < \theta < \pi$, and the transformation $h^{sc+}_{l,\theta}(k,r) = r^{l+1}\psi^{sc+}_{l,\theta}(k,r)$, which results in a regular function $h^{sc+}_{l,\theta}(k,r)$ at $r = 0$) we get the driven radial Schrödinger equation

$$\left[\frac{k^2}{2} + e^{-2i\theta}\frac{1}{2}\frac{d^2}{dr^2} - e^{-2i\theta}\frac{l}{r}\frac{d}{dr} - e^{-i\theta}\frac{\gamma k}{r} - V_s(re^{i\theta})\right] h^{sc+}_{l,\theta}(k,r) = r^{l+1}S^{tot}_{l,\theta}(k,r), \tag{9}$$

where the new source term reads

$$S^{tot}_{l,\theta}(k,r) = S_{l,\theta}(k,r) + e^{i3\theta/2}\psi_{i,l}(k,re^{i\theta})V_s(re^{i\theta}). \tag{10}$$

The boundary conditions are

$$h^{sc+}_{l,\theta}(k,0) = 0 \tag{11}$$

and

$$\lim_{r\to\infty} h^{sc+}_{l,\theta}(k,r) = 0. \tag{12}$$

One can show that the phase shift δ_l can be expressed as the $r \to \infty$ limit of a function $\sigma_l(r)$, which we call the local representation of the phase shift:

$$e^{2i\sigma_l(r)} = (2kre^{i\theta})^{i\gamma}\left[e^{-ikre^{i\theta}}2ikre^{-i\theta/2}\tilde{\psi}^{sc+}_{l,\theta}(k,r) + \frac{e^{\gamma\pi/2}(-1)^l(i\gamma-l)_l}{\Gamma(l+1-i\gamma)}\right] \to e^{2\delta_l} \quad (r\to\infty). \tag{13}$$

3. Numerical Results

In numerical calculations the boundary condition (12) is approximated by a similar expression for a large but finite value R of r, which in in the asymptotic region:

$$h^{sc+}_{l,\theta}(k,R) = 0. \tag{14}$$

The finite element method is used as a numerical technique for the solution of Eq. (9). In the calculations equally spaced finite elements of length 1 atomic unit are taken. The degree of the Lobatto shape functions is denoted by N, and the same N value is chosen for each element. A short-range potential $V_s = 7.5r^2\exp(-r)$ is added to the Coulomb potential.

In Figure 1 a case of $\theta = 0.1$ radian is shown, with the angular momentum $l = 0$ and $k = 3$. The Coulomb potential is given by $1/r$. The local representation of the phase shift is practically constant in a huge region, which can be identified with an approximate phase-shift value. In contrast the local approximation of the phase shift in [5] tends to the exact value by a persistent oscillation with decreasing order of amplitude.

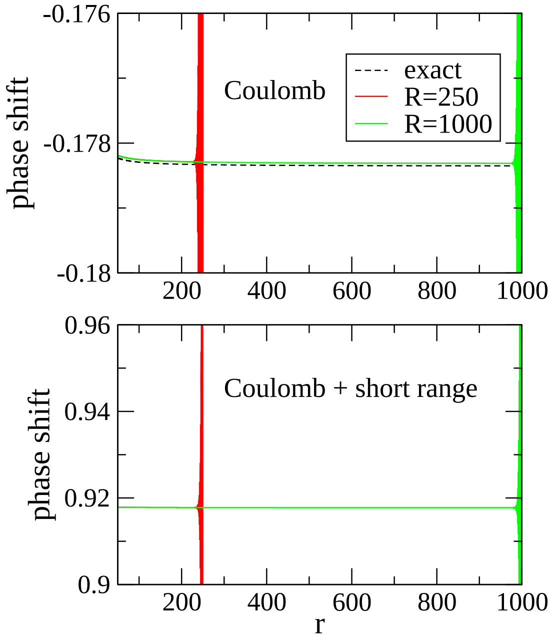

Figure 1. The local representation of the phase shift for the pure Coulomb potential (upper part) and for the Coulomb plus short-range potential (lower part). For the pure Coulomb case the dashed line displays the exact solution.

4. Conclusion

The two-body scattering problem has been solved for a pure Coulomb potential as well as for a Coulomb plus finite-range potential using the standard complex scaling method. No cutoff is applied to the tail of the long-range interaction. The CS makes it possible to observe the scattering boundary condition with great accuracy in a fairly simple manner.

Reference

[1] Hornyak I and Kruppa A T 2012 *Phys. Rev.* A **85** 022702
[2] Rescigno T N, Baertschy M, Byrum D and McCurdy C W 1997 *Phys. Rev.* A **55** 4253
[3] Kruppa A T, Suzuki R and Kato K 2007 *Phys. Rev.* C **75** 044602
[4] van Haeringen H 1976 *Il Nuovo Cimento* **34B** 53
[5] Volkov M V, Elander N, Yarevsky E and Yakovlev S L 2009 *Europhys. Lett.* **85** 30001