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Scattering in the \mathcal{PT} -symmetric Coulomb potential

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Abstract

Scattering on the \mathcal{PT} -symmetric Coulomb potential is studied along a U-shaped trajectory circumventing the origin in the complex x plane from below. This trajectory reflects \mathcal{PT} symmetry, sets the appropriate boundary conditions for bound states and also allows the restoration of the correct sign of the energy eigenvalues. Scattering states are composed from the two linearly independent solutions valid for non-integer values of the $2L$ parameter, which would correspond to the angular momentum in the usual Hermitian setting. The transmission and reflection coefficients are written in a closed analytic form, and it is shown that, similar to other \mathcal{PT} -symmetric scattering systems, the latter exhibit the handedness effect. Bound-state energies are recovered from the poles of the transmission coefficients.

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1. Introduction

The Kepler–Coulomb problem has always played a special role in the formulation and application of quantum mechanics. Besides being one of the textbook examples for exactly solvable problems, it also exhibits features that have always attracted the attention of mathematical physicists. Among these one can mention that the Coulomb potential possesses both discrete and continuous spectra, which can be associated with dynamical symmetry and Lie algebras describing them (see e.g. [1] for a review). Although in the description of realistic physical systems the three-dimensional Coulomb potential and the associated radial Schrödinger equation are used in most cases, much work has been done extending the Coulomb potential to other dimensions. Of these, the one-dimensional Coulomb potential is the most notable, as the singularity at $x = 0$ raises interesting questions both for the $V(x) \sim -x^{-1}$ and $V(x) \sim -|x|^{-1}$ potentials (see e.g. [2] and references therein). The discussion of this

seemingly humble system requires techniques like the self-adjoint extension of the relevant differential operator [3].

Manifestly non-Hermitian versions of the Coulomb potential have also been studied in terms of \mathcal{PT} -symmetric quantum mechanics. In this theory [4], Hamiltonians invariant with respect to the simultaneous \mathcal{P} space and \mathcal{T} time inversion were found to exhibit characteristic features of Hermitian systems, such as partly or fully real energy spectrum and the conservation of the norm (see e.g. [5] for a recent review).

The first examples for \mathcal{PT} -symmetric potentials were of the type $V(x) = x^2(ix)^\epsilon$, including the archetypal imaginary cubic potential for $\epsilon = 1$. After the first numerical results, the conjecture of the reality of the energy spectrum was proven analytically for such potentials [6]. An interesting aspect of these systems is that often they cannot be defined on the real x -coordinate axis, rather their solutions are normalizable only along certain trajectories of the complex x plane. This was the case, for example, for the above potential with $\epsilon \geq 2$, when these trajectories had to fall into wedges lying in the lower half of the plane in ϵ -dependent positions symmetrical with respect to the imaginary axis.

Later the \mathcal{PT} -symmetric version of a number of exactly solvable potentials was formulated, mainly along the real x -axis or along a line parallel with it $x - ic$ (see e.g. [7] and references therein). The importance of this imaginary shift was that singularities lying on the real x -axis could be avoided and, at the same time, the energy spectrum remained independent of c . In this way, real potentials defined on the positive half-axis could be extended to negative x values too. As a result of this, solutions irregular in the Hermitian case became regular in the \mathcal{PT} -symmetric version of the potential, and this led to a richer energy spectrum.

The Coulomb potential was among the first exactly solvable potentials considered within the \mathcal{PT} -symmetric setting. It was found, however, that it cannot be defined on the real x -axis because the solutions are not regular for both $x \rightarrow \infty$ and $x \rightarrow -\infty$ [7]. In [8] a parabolic trajectory was proposed, which was inspired by the \mathcal{PT} -symmetrized version of the well-known harmonic oscillator–Coulomb mapping. This study revealed that the spectrum of the \mathcal{PT} -symmetric Coulomb potential includes a second set of discrete energy eigenvalues in addition to the one that is present also in the spectrum of the real Coulomb potential. But as a more interesting feature, the energy spectrum was inverted [8]. The interpretation of this unusual finding was given later in [9]. The transformation properties of the solutions under the \mathcal{PT} operation including solutions both with real and pairwise complex conjugate energy eigenvalues were also discussed [10]. Another study of the \mathcal{PT} -symmetric Coulomb potential was done in [11]: there the Coulomb potential was defined as $V(x) \sim |x - ic|^{-1}$.

In the present work we extend, to the scattering scenario, the discussion of the \mathcal{PT} -symmetric Coulombic bound states as presented in [8, 9]. In this direction we intend to pursue two ideas. The first one reflects the existence of a number of publications [12–16] where the standard \mathcal{PT} -symmetric version of the scattering problem has already been described and developed in application to a number of exactly solvable potentials. We feel inspired by the observation that in all of these works the scattering has only been considered along the real x -axis and/or along a trivially complexified, shifted straight-line contour $x(s) = s - ic$ with a real variable s and constant c . We shall change this perspective by employing an utterly nontrivial negative-mass generalization of the complex integration path $x = x_{(\epsilon)}^U(s)$ as already proposed, in the context of the stabilization of the Coulomb-bound states in [9] (see also equation (5) below). In this setting, we shall reveal the new role of the real parameter ϵ which indeed appears to bring a new degree of freedom in the phenomenological scattering theory.

The second motivation for our present interest in the \mathcal{PT} -symmetric Coulombic scattering along a U-shaped contour $x(s)$ given in [9] is more physical since it reflects the unique possibility of the *coexistence* of discrete and scattering states in a single potential (in this

respect cf, e.g., the review [1] once more). We have to emphasize that in the \mathcal{PT} -symmetric context such a feature has not yet been achieved, even in the models of scattering along curved–complex contours (cf, e.g., [17] where the ‘tobogganic’ integration path $x = x(s)$ has been chosen as extending, in principle, along several Riemann sheets of the scattering wavefunctions $\psi(x(s))$). Thus, the present U-shaped choice of $x_{(\varepsilon)}^U(s)$ will represent the physics which varies with the ‘contour width’ ε . This seems to offer a scattering-scenario analogue of the variability of the bound-state spectra mediated, according to [4, 17], by the variability of our choice of Stokes’ ‘wedges’ in the complex x plane.

The structure of the paper is as follows. In section 2, the general formulation of the problem is presented together with the U-shaped trajectory along which the scattering problem is considered. Section 3 deals with the actual calculation of the transmission and reflection coefficients, while the results are summarized in section 4.

2. Definition of the problem

Let us consider the Schrödinger equation

$$\frac{\hbar^2}{2m} \left[-\frac{d^2}{dx^2} + \frac{L(L+1)}{x^2} \right] \Psi(x) + V(x)\Psi(x) = E\Psi(x), \quad (1)$$

defined in the x variable, which runs along a trajectory of the complex x plane. Let us assume that this trajectory can be parametrized in terms of a real variable as $x(s)$. In order to implement \mathcal{PT} symmetry of this system, we introduce

$$V(x) = \frac{iZ}{x}, \quad (2)$$

where Z and $L(L+1)$ are real. This latter condition is met if L is chosen real. The two linearly independent solutions of (1) can be written in terms of the confluent hypergeometric functions as

$$\Psi_1(x) = C_1 e^{-kx} x^{L+1} {}_1F_1(1+L+iZ/(2k), 2L+2, 2kx), \quad (3)$$

$$\Psi_2(x) = C_2 e^{-kx} x^{-L} {}_1F_1(-L+iZ/(2k), -2L, 2kx), \quad (4)$$

where $2mE/\hbar^2 = -k^2$. Note that (3) and (4) represent the two linearly independent solutions only if $2L \notin \mathbb{Z}$.

Equation (1) with (2) differs from the usual radial Schrödinger equation of the Coulomb problem in the complexified potential, and also in the trajectory it is defined on. In a systematic reformulation of real solvable potentials and the respective bound states to their \mathcal{PT} -symmetric counterpart it was found [7] that this problem cannot be defined on the real x -axis or its imaginary shifted version $x - ic$, because the boundary conditions cannot be implemented in both directions due to the exponential factor in (3) and (4). In an effort to determine the genuine \mathcal{PT} -symmetric version of the Coulomb potential, the well-known Coulomb-harmonic oscillator mapping was used: this transformation was applied to the \mathcal{PT} -symmetric harmonic oscillator defined on the imaginary shifted real axis $x - ic$ [8]. The resulting trajectory was a parabola in the first and fourth quadrants, circumventing the origin from the left. In order to make it \mathcal{PT} -symmetric, i.e. left–right symmetric in the coordinate space, it had to be tilted to the first and second quadrants by the multiplication of ix . In order to keep the kx quantity intact, k also had to be tilted in the opposite direction in the k wave number space as $-ik$. This resulted in the unusual finding that the energy spectrum was inverted, as can be seen from the relation $2mE/\hbar^2 = -k^2$. Note that the two sets of discrete-energy solutions discussed in [8]

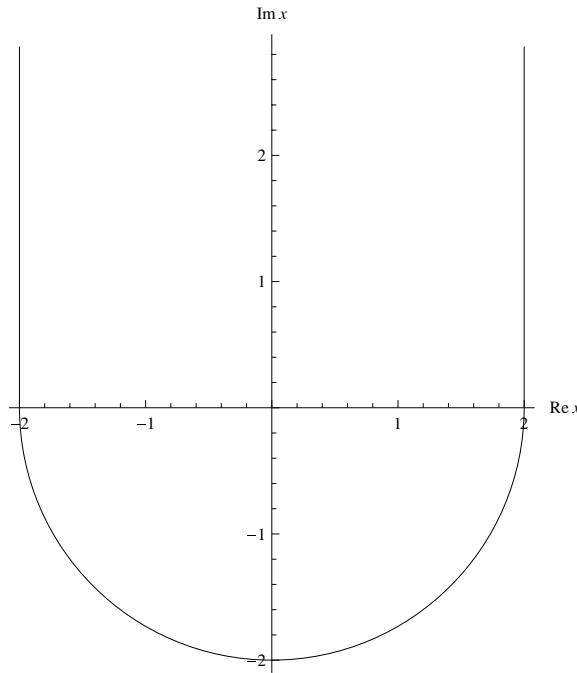


Figure 1. The U-shaped curve in a complex x plane for $\varepsilon = 2$

are obtained from (3) and (4) by substituting a non-positive integer in the first argument of the respective confluent hypergeometric functions, reducing them to the expected generalized Laguerre polynomial form [18]. (In order to match the formulae of [8] with those obtained here, the following substitutions have to be made: $t \rightarrow x$, $A \rightarrow L + 1/2$, $e^2 = 1$, while κ^2 should be chosen as $Z/[2(n + L + 1)]$ and $Z/[2(n - L)]$ in the two cases, corresponding to the two possible values of the quasi-parity $q = \pm 1$.)

As another possible trajectory, a U-shaped curve circumventing the origin, illustrated in figure 1, was proposed in [9]. It is defined for a suitable $\varepsilon > 0$ as

$$x(s) = x_{(\varepsilon)}^U(s) = \begin{cases} -i(s + \frac{\pi}{2}\varepsilon) - \varepsilon, & s \in (-\infty, -\frac{\pi}{2}\varepsilon), \\ \varepsilon e^{i(s/\varepsilon + 3/2\pi)}, & s \in (-\frac{\pi}{2}\varepsilon, \frac{\pi}{2}\varepsilon), \\ i(s - \frac{\pi}{2}\varepsilon) + \varepsilon, & s \in (\frac{\pi}{2}\varepsilon, \infty). \end{cases} \quad (5)$$

The asymptotic ε dependence of this curve has an immediate physical meaning because it enables us to distinguish between non-equivalent alternative asymptotes of the curves $x(s)$ along which the non-equivalent asymptotic boundary conditions will be specified for our wavefunctions. Of course, in contrast to the scattering wavefunctions, which must be different on the left and right asymptotic branches of $x(s)$, all of the curves of coordinates exhibit the same left–right symmetry $x(-s) = -x^*(s)$ in the complex x plane, which combines spatial reflection \mathcal{P} with complex conjugation \mathcal{T} that mimics time reversal. It is seen that for the large $|s|$ (in fact, for $|s| \gg \varepsilon\pi/2$), the solutions behave as $\exp(\pm ik|s|)$. For real $k = (-2mE)^{1/2}/\hbar$ (i.e. for $m > 0$ and $E < 0$ of [8] or for $m < 0$ and $E > 0$ in [9]), this represents an oscillatory solution. In parallel, for an imaginary k (i.e. for $m > 0$ and $E > 0$ or for $m < 0$ and $E < 0$), it corresponds to exponentially decaying or growing solutions, depending on the sign of $\text{Im}(k)$.

The next result of this analysis, presented also in [9], is that at the negative mass, the U-shaped parametrization (5) opens the way towards the *simultaneous* description of the bound and scattering states. In this setting, the role of the asymptotic physical coordinate is played by the real parameter s of course.

The matching of logarithmic derivatives is usually used in models where the potential V is, at some point $x(s_0)$ of the curve of (possibly, complexified) coordinates, discontinuous. For analytic potentials (leading to analytic wavefunctions $\psi(x)$), the situation is different since these functions are usually well defined in all the points of some Riemann surface \mathcal{S} . This means that, in general, our analytic wavefunctions are multi-valued functions which become single-valued, typically, on any selected Riemann sheet specified, say, as a subdomain \mathcal{D} of a cut complex plane \mathbb{C} . In such a scenario, it is only necessary to match the logarithmic derivatives of our analytic wavefunctions $\psi(x(s))$ during transition of the path $x(s)$ between neighbouring Riemann sheets of the Riemann surface (i.e. typically, between the pairs of non-overlapping subdomains \mathcal{D}_\pm of \mathbb{C}). For this purpose, it is usually sufficient to employ the analyticity of $\psi(x)$ and to simplify the matching via a suitable deformation of the path $x(s)$. Thus, most easily, one may analyse the transition between \mathcal{D}_+ and \mathcal{D}_- just in an arbitrarily small vicinity of a branch point where functions $\psi(x)$ degenerate to their dominant parts with trivial analytic-continuation properties.

3. Scattering in the \mathcal{PT} -symmetric Coulomb potential

In what follows, we shall make use of the parametrization (5) to study scattering on the \mathcal{PT} -symmetric Coulomb potential at negative mass. In [9] this unusual option has been explained as making the \mathcal{PT} -symmetric Coulomb-bound states stable. Here, we shall emphasize that such an option is also necessary for a consistent description of the scattering along the U-shaped complex contour.

On a purely technical level, we shall employ the natural analytic continuity of functions (3) and (4). In order to facilitate the implementation of this idea, the auxiliary complex phase factors $\exp(2\pi i(L+1))$ and $\exp(2\pi i(-L))$ will be introduced in the two solutions for $\text{Re}(x) > 0$. Then, the asymptotic expansion of the solutions can be written as [19]

$$\begin{aligned}
 {}_1F_1(a, b, z) \sim & \frac{\Gamma(b)}{\Gamma(b-a)} (z^{-1} e^{i\pi})^a {}_2F_0(a, 1+a-b, -z^{-1}) \\
 & + \frac{\Gamma(b)}{\Gamma(a)} e^z z^{a-b} {}_2F_0(b-a, 1-a, z^{-1}),
 \end{aligned} \tag{6}$$

where $\text{Im}(z) > 0$, $|\text{Arg}(z)| < \pi$ as $|z| \rightarrow \infty$.

Applying (6) to (3) and (4) and employing the parametrization of x (5), the following asymptotic expansions are obtained for $|s| \rightarrow \infty$:

$$\begin{aligned}
 \psi_j(s \rightarrow -\infty) \sim & a_{j-} e^{i(k s - \frac{Z}{2k} \ln(-2ks))} + b_{j-} e^{-i(k s - \frac{Z}{2k} \ln(-2ks))}, \\
 \psi_j(s \rightarrow \infty) \sim & a_{j+} e^{i(k s + \frac{Z}{2k} \ln(2ks))} + b_{j+} e^{-i(k s + \frac{Z}{2k} \ln(2ks))},
 \end{aligned} \tag{7}$$

where $j = 1, 2$. The logarithmic terms in the exponentials are characteristic of the Coulomb asymptotics and indicate that the Coulomb potential vanishes slower than genuine short-range potentials exhibiting the exponential tail, for example [20]. The coefficients are

$$a_{1+} = C_1 (2k)^{-L-1} e^{-ik\pi\epsilon/2} e^{i\pi(2L+2)} e^{-\frac{\pi Z}{4k}} e^{k\epsilon} \frac{\Gamma(2L+2)}{\Gamma(L+1+iZ/(2k))}, \tag{8}$$

$$a_{1-} = C_1 (2k)^{-L-1} e^{ik\pi\epsilon/2} e^{i\pi(L+1)} e^{-\frac{\pi Z}{4k}} e^{k\epsilon} \frac{\Gamma(2L+2)}{\Gamma(L+1-iZ/(2k))}, \tag{9}$$

$$b_{1+} = C_1(2k)^{-L-1} e^{ik\pi\epsilon/2} e^{i\pi(3L+3)} e^{-\frac{\pi Z}{4k}} e^{-k\epsilon} \frac{\Gamma(2L+2)}{\Gamma(L+1-iZ/(2k))}, \quad (10)$$

$$b_{1-} = C_1(2k)^{-L-1} e^{-ik\pi\epsilon/2} e^{-\frac{\pi Z}{4k}} e^{-k\epsilon} \frac{\Gamma(2L+2)}{\Gamma(L+1+iZ/(2k))}, \quad (11)$$

$$a_{2+} = C_2(2k)^L e^{-ik\pi\epsilon/2} e^{i\pi 2L} e^{-\frac{\pi Z}{4k}} e^{k\epsilon} \frac{\Gamma(-2L)}{\Gamma(-L+iZ/(2k))}, \quad (12)$$

$$a_{2-} = C_2(2k)^L e^{ik\pi\epsilon/2} e^{-i\pi L} e^{-\frac{\pi Z}{4k}} e^{k\epsilon} \frac{\Gamma(-2L)}{\Gamma(-L-iZ/(2k))}, \quad (13)$$

$$b_{2+} = C_2(2k)^L e^{ik\pi\epsilon/2} e^{-i\pi 3L} e^{-\frac{\pi Z}{4k}} e^{-k\epsilon} \frac{\Gamma(-2L)}{\Gamma(-L-iZ/(2k))}, \quad (14)$$

$$b_{2-} = C_2(2k)^L e^{-ik\pi\epsilon/2} e^{-\frac{\pi Z}{4k}} e^{-k\epsilon} \frac{\Gamma(-2L)}{\Gamma(-L+iZ/(2k))}. \quad (15)$$

Note that as expected from the functional form of the solutions, the interchange of the indices $1 \leftrightarrow 2$ corresponds to the interchange $L \leftrightarrow -L - 1$. These coefficients are also connected by the expressions

$$b_{1+} = a_{1-} e^{-2k\epsilon} e^{2i\pi(L+1)}, \quad b_{1-} = a_{1+} e^{-2k\epsilon} e^{-2i\pi(L+1)}, \quad (16)$$

$$b_{2+} = a_{2-} e^{-2k\epsilon} e^{2i\pi(-L)}, \quad b_{2-} = a_{2+} e^{-2k\epsilon} e^{2i\pi L}. \quad (17)$$

The asymptotic expansion of the general wavefunction $\Phi(x(s)) = \alpha\psi_1(x(s)) + \beta\psi_2(x(s))$ is then the following:

$$\Phi(s \rightarrow -\infty) \sim (\alpha a_{1-} + \beta a_{2-}) e^{i(k s - \frac{Z}{2k} \ln(-2ks))} + (\alpha b_{1-} + \beta b_{2-}) e^{-i(k s - \frac{Z}{2k} \ln(-2ks))}, \quad (18)$$

$$\Phi(s \rightarrow \infty) \sim (\alpha a_{1+} + \beta a_{2+}) e^{i(k s + \frac{Z}{2k} \ln(2ks))} + (\alpha b_{1+} + \beta b_{2+}) e^{-i(k s + \frac{Z}{2k} \ln(2ks))}. \quad (19)$$

In the following step, we may construct solutions that correspond to an incoming wave from one direction in order to evaluate the reflection and transmission coefficients [16]. Using the coefficients above, the following results are obtained after some manipulations with gamma, trigonometric and exponential functions:

$$T_{L \rightarrow R}(k) = \frac{i}{2\pi} e^{-i\pi k\epsilon} e^{\frac{\pi Z}{2k}} \Gamma(-L - iZ/(2k)) \Gamma(L + 1 - iZ/(2k)), \quad (20)$$

$$R_{L \rightarrow R}(k) = T_{L \rightarrow R}(k) e^{-2k\epsilon} \left(-e^{-\frac{\pi Z}{k}} + 2 \cos(2\pi L) \right), \quad (21)$$

$$T_{R \rightarrow L}(k) = -T_{L \rightarrow R}(k), \quad (22)$$

$$R_{R \rightarrow L}(k) = T_{R \rightarrow L}(k) e^{2k\epsilon} e^{-\frac{\pi Z}{k}}. \quad (23)$$

It is seen that, as expected, the bound-state energies emerge from the poles of $T_{L \rightarrow R}(k)$ (20), i.e. when the arguments of the gamma functions are set to the $-n$ non-positive integer.

Equation (22) is also in accordance with the results of scattering on other \mathcal{PT} -symmetric potentials in that the transmission coefficient does not show the handedness effect, except for a trivial factor of -1 , while the reflection coefficients clearly demonstrate handedness [14, 16]. This means that, similar to other examples, waves arriving from the asymptotically absorptive side scatter differently from waves arriving from the asymptotically emissive one.

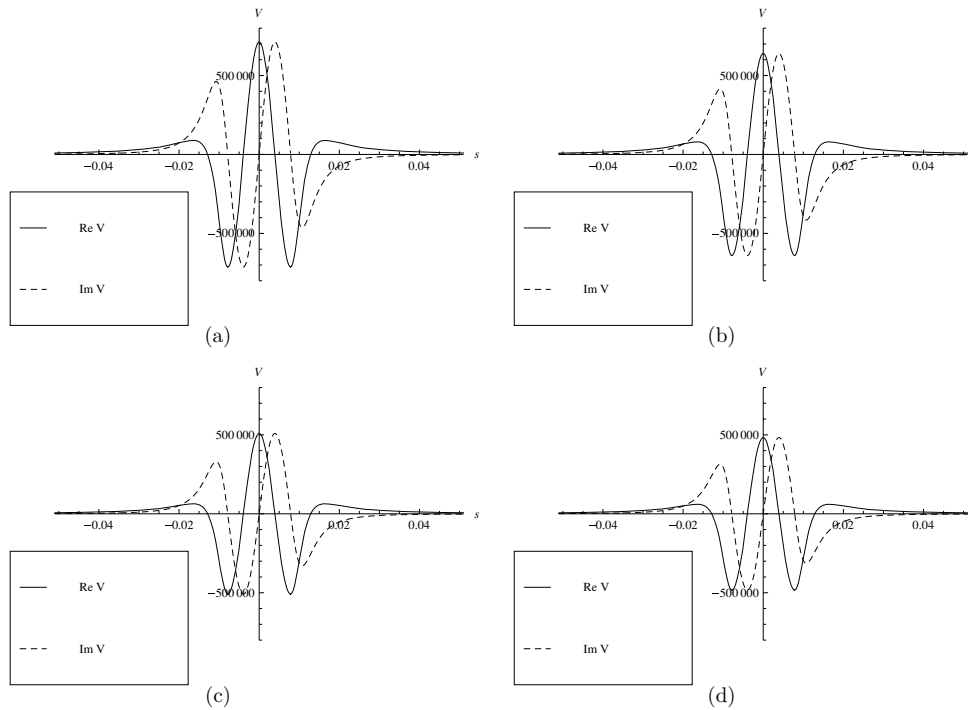


Figure 2. The \mathcal{PT} -symmetric Coulomb potential plotted as the function of s parameter for $Z = 1$, $\varepsilon = 0.005$, and (a) $L = 3.75$, (b) $L = 3.53$, (c) $L = 3.10$, (d) $L = 3.01$.

To exemplify the results, we present in figure 2 the potential as the function of s for some parameters, together with the transmission and reflection coefficients in figure 3 for a series of parameters. As expected, the real and the imaginary potential components are even and odd functions of s ; furthermore, the real component decays quicker than the imaginary one as it should be based on (1). The role of the ε parameter is essentially that of a length scale. L and Z set the scale of the real and imaginary potential components, respectively.

It is seen that the large- k behaviour of $T_{L \rightarrow R}(k)$ is relatively smooth, while those of the reflection coefficients are dominated by the $\exp(\pm 2k\varepsilon)$ factors. An exception for this behaviour is seen only near integer values of L , which are excluded from the present discussion. The Z ‘charge’ parameter does not influence the results in an essential way.

4. Summary

Scattering on the \mathcal{PT} -symmetric Coulomb potential was discussed on a trajectory of the complex x plane. This trajectory was a U-shaped curve circumventing the origin from below, guaranteeing the asymptotical regularity of bound states. From the topological point of view, it is similar to the parabolic path obtained from the application of the harmonic oscillator–Coulomb mapping of bound states to the \mathcal{PT} -symmetric setting [8]. It is also reminiscent to the trajectories obtained by similar regularity arguments for the power-type potentials appearing in the first publications of \mathcal{PT} -symmetric quantum mechanics [4]: there the allowed wedges for the solutions were located in the lower half of the complex x plane, while here the allowed domain is the upper half, corresponding formally to the inverted power $(ix)^{-1}$ expression of the Coulomb potential. In addition to the Coulombic potential term, a centrifugal-like term

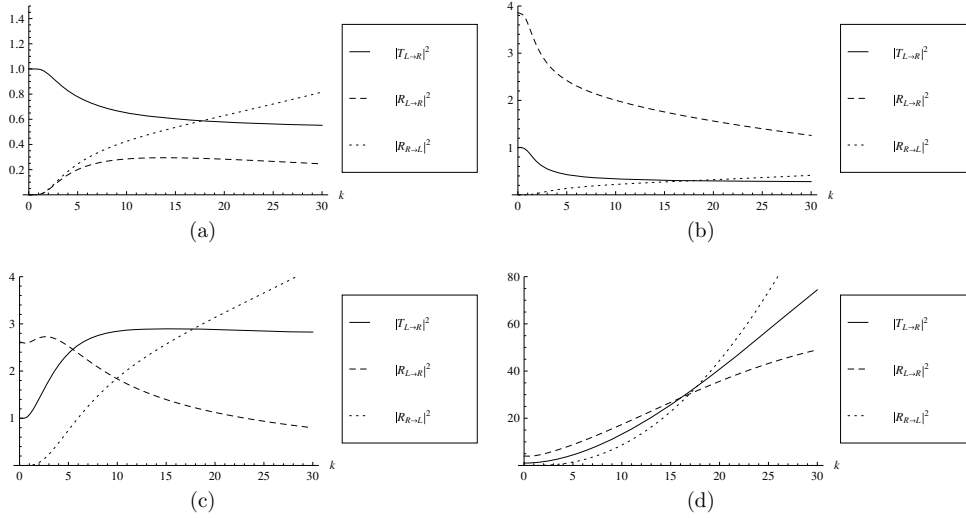


Figure 3. Transmission and reflection coefficients for $Z = 1$, $\varepsilon = 0.005$, and (a) $L = 3.75$, (b) $L = 3.53$, (c) $L = 3.10$, (d) $L = 3.01$.

$L(L + 1)x^{-2}$ was also considered. Here integer values of L were excluded, because in that case the linearly independent solutions had to be defined in another way.

Parametrizing the trajectory as $x(s)$ in terms of the real parameter $s \in (-\infty, \infty)$ allowed the expression of the asymptotic solutions in a form familiar from the discussion of the real Coulomb potential. When parametrized in terms of s , the real and the imaginary potential components vanished as s^{-2} and s^{-1} , i.e. the imaginary potential component dominates the problem asymptotically.

The transmission and reflection coefficients were determined, from the asymptotic solutions, with special attention to the continuity of the solutions in the complex plane. It was found that the transmission coefficients for waves arriving from the two directions differ only in a trivial factor of -1 , while the reflection coefficients exhibit manifest handedness. This is similar to other examples for scattering in \mathcal{PT} -symmetric potentials, which, however, were defined on the real x -axis or its trivial shifted version $x - ic$. The ε parameter appearing in the definition of the U-shaped curve plays a role similar to the c parameter applied in [12, 13] to shift the trajectory off the real x -axis. Although it changes the potential shape, it does not influence the energy spectrum.

The results showed strong dependence on the ε parameter that sets the distance of the U-shaped trajectory from the positive imaginary axis, while the Z ‘charge’ parameter did not influence the results in an essential way. It essentially sets the relative weight of the imaginary and real potential components. Dependence on the L parameter was also significant in that the transmission and reflection coefficients showed rapid variations close to the forbidden integer values of L .

As another aspect similar to other scattering problems, both Hermitian and \mathcal{PT} -symmetric, the two sets of bound-state energy eigenvalues described in [8] could be recovered from the poles of the transmission coefficients. Furthermore, the reparametrization of the problem in terms of the s variable also allowed us to recover the energy spectrum with the correct sign: $E < 0$ for bound states and $E > 0$ for scattering states.

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