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Spontaneous breakdown of $\mathcal{PT}$ symmetry in the complex Coulomb potential

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Abstract. The $\mathcal{PT}$ symmetry of the Coulomb potential and its solutions are studied along trajectories satisfying the $\mathcal{PT}$ symmetry requirement. It is shown that with appropriate normalization constant the general solutions can be chosen $\mathcal{PT}$-symmetric if the L parameter that corresponds to angular momentum in the Hermitian case is real. $\mathcal{PT}$ symmetry is spontaneously broken, however, for complex L values of the form $L = -\frac{1}{2} + \mathrm{i}\lambda$. In this case the potential remains $\mathcal{PT}$-symmetric, while the two independent solutions are transformed to each other by the $\mathcal{PT}$ operation and at the same time, the two series of discrete energy eigenvalues turn into each other's complex conjugate.

Keywords. Spontaneous breakdown of $\mathcal{PT}$ symmetry; Coulomb potential; complex energy eigenvalues.

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1. Introduction

One of the most intriguing features of $\mathcal{PT}$-symmetric quantum mechanics is the spontaneous breakdown of $\mathcal{PT}$ symmetry. This phenomenon was noted in the first examples for $\mathcal{PT}$-symmetric systems, i.e. the power-type potentials $V(x) = x^2(\mathrm{i}x)^\varepsilon$ proposed by Bender and Boettcher [1]. It was observed that for $\varepsilon > 0$ all the energy eigenvalues are real (later this was proven analytically [2]), while for $\varepsilon < 0$ the real energy eigenvalues merge pairwise and re-appear as complex conjugate pairs. This mechanism was interpreted as the spontaneous breakdown of $\mathcal{PT}$ symmetry, because at the same time the eigenfunctions of the Hamiltonian ceased to be the eigenfunctions of the $\mathcal{PT}$ operator, while the $\mathcal{PT}$ symmetry of the Hamiltonian itself remained intact.

Later the mechanism of the spontaneous breakdown of $\mathcal{PT}$ symmetry was studied in a number of exactly solvable potentials [3–5] and it was found that the complexification of the energy spectrum typically occurs when the non-Hermiticity of the Hamiltonian increases. After the systematic study of the most well-known, i.e. shape-invariant potentials, the mechanism of the spontaneous breakdown of $\mathcal{PT}$

symmetry was studied for more general solvable potentials from the Natanzon-class [6,7] and beyond [8].

The Coulomb potential was among the first shape-invariant potentials studied in terms of the $\mathcal{PT}$-symmetric setting [9]. It turned out, however, that it cannot be defined on the real x-axis [10], rather, in order to obtain normalizable energy eigenfunctions the problem has to be defined on some trajectories of the complex x plane. This showed similarity with the power-type potentials of Bender and Boettcher [1], which had to be defined along curves falling into ϵ-dependent wedges in the lower half of the complex x plane. In the case of the Coulomb potential the trajectory was also left–right symmetric in the complex plane, but it had to be defined on the upper half of the plane. It also turned out that the energy spectrum was inverted. To rectify this problem, a U-shaped trajectory was proposed in ref. [11], in the complex plane, which was parametrized in terms of a real variable. With this, not only was it possible to restore the correct sign of the energy spectrum, but also scattering solutions of the $\mathcal{PT}$-symmetric Coulomb problem could be described, together with the transmission and reflection coefficients [12]. Despite the unusual setting of this potential, the results for the transmission and reflection coefficients showed a behaviour similar to that observed for potentials defined on the real x-axis: the latter showed manifest handedness effect, while the former one did not [13,14].

The $\mathcal{PT}$-symmetric Coulomb potential showed similarity to a number of other $\mathcal{PT}$-symmetric potentials in that it had two sets of discrete solutions distinguished by the quasi-parity quantum number $q = \pm 1$ [3,15]. The second set of the solutions typically arose by the regularization of the singularities of the potential along the real x-axis by the imaginary coordinate shift $x - \mathrm{i}c$ [3,16], although they appeared for the non-singular Scarf II potential: in that case the second set of solutions evolved from solutions that corresponded to resonances in the Hermitian setting [4,17]. It was also seen that during the spontaneous breakdown of $\mathcal{PT}$ symmetry the pair of energy eigenvalues turning into complex conjugate pairs were states carrying the same principal quantum number n, but opposite quasi-parity.

Our present study is motivated by the fact that complex-energy solutions of the $\mathcal{PT}$-symmetric Coulomb potential have not been studied, only real-energy bound-state and scattering solutions. Here we plan to fill this gap and also investigate the similarities and differences between the mechanism of spontaneous breakdown of $\mathcal{PT}$ symmetry in the Coulomb and other solvable potentials.

2. Conditions for $\mathcal{PT}$ symmetry

Let us consider the Schrödinger equation

$$\frac{\hbar^2}{2m}\left[-\frac{\mathrm{d}^2}{\mathrm{d}t^2}+\frac{L(L+1)}{t^2}\right]\Psi(x)+\frac{\mathrm{i}Z}{t}\,\Psi(t)=E\,\Psi(t)\,, \tag{1}$$

defined in the t variable, which runs along a trajectory of the complex t plane. Let us assume that this trajectory can be parametrized in terms of a real variable $x \in (-\infty, \infty)$ such that it obeys

$$t^*(-x) = -t(x) \tag{2}$$

relation. If x runs along the real t-axis, then the trajectory is left–right symmetric in the complex t plane with respect to the imaginary axis, i.e. it is $\mathcal{PT}$-symmetric. Let us consider the potential

$$V_C(x) = \frac{L(L+1)}{t^2(x)} + \frac{\mathrm{i}Z}{t(x)}\,, \tag{3}$$

containing the terms, which, for non-negative integer L values would correspond formally to the Coulomb and centrifugal terms in radial Schrödinger equation of the usual Hermitian Coulomb problem. Here we allow more general values for L, so the problem is a generalization of the Kratzer potential.

From (2) it follows that $V_C(x)$ is $\mathcal{PT}$-symmetric if Z and $L(L+1)$ are real. The latter condition is satisfied if L is either real or has the complex form $L = -\frac{1}{2} + \mathrm{i}\lambda$, where λ is real. The conditions mentioned up to now do not guarantee automatically the $\mathcal{PT}$ symmetry and the normalizability of the solutions. So further study of the solutions of this problem is necessary. In what follows we consider the U-shaped trajectory proposed in ref. [11]:

$$t(x) = x^U_{(\varepsilon)}(x) \;=\; \begin{cases} -\mathrm{i}(x + \frac{\pi}{2}\varepsilon) - \varepsilon, & x \in (-\infty, -\frac{\pi}{2}\varepsilon), \\ \varepsilon \mathrm{e}^{\mathrm{i}(x/\varepsilon + 3\pi/2)}, & x \in (-\frac{\pi}{2}\varepsilon, \frac{\pi}{2}\varepsilon), \\ (\mathrm{i}(x - \frac{\pi}{2}\varepsilon) + \varepsilon)\,, & x \in (\frac{\pi}{2}\varepsilon, \infty). \end{cases} \tag{4}$$

Here $\varepsilon > 0$ is assumed. This trajectory circumvents the origin from below and is symmetric with respect to the imaginary axis. With this choice the sign of the kinetic energy term (i.e. that of the mass) could be inverted and the bound-state energy spectrum that had wrong sign in ref. [9] could be restored to the more natural negative domain.

2.1 *The linearly independent solutions*

If $2L$ is not an integer, then the two linearly independent solutions of (1) can be written in terms of confluent hypergeometric functions [18] as

$$\Psi_1(x) = C_1\,\mathrm{e}^{-kt(x)}(t(x))^{L+1}{}_1F_1(1 + L + \mathrm{i}Z/(2k), 2L + 2, 2kt(x)) \tag{5}$$

$$\Psi_2(x) = C_2\,\mathrm{e}^{-kt(x)}(t(x))^{-L}{}_1F_1(-L + \mathrm{i}Z/(2k), -2L, 2kt(x)), \tag{6}$$

where

$$E = -\frac{\hbar^2 k^2}{2m} \tag{7}$$

from (1). Introducing the notation

$$\omega(q, L) = \frac{1}{2} + q\left(L + \frac{1}{2}\right) \tag{8}$$

with $q = \pm 1$ the two solutions (5) and (6) can be written in a compact form

$$\Psi_q(x) = C_q \,\mathrm{e}^{-kt(x)}(t(x))^{\omega(q,L)}{}_1F_1(\omega(q,L) + \mathrm{i}Z/(2k), 2\omega(q,L), 2kt(x)). \tag{9}$$

Here the q parameter plays the role of quasi-parity [3,15], similar to some other solvable $\mathcal{PT}$-symmetric potentials. Note that

$$\omega^*(q,L) = \omega(q,L^*). \tag{10}$$

From the point of view of the asymptotic behaviour of (9) the exponential factor $\mathrm{e}^{-kt(x)}$ is crucial. With the parametrization (4) it is asymptotically $\exp(-\mathrm{i}k|x|)$, i.e. for real values of k it is an oscillatory function, while for imaginary k it decays or increases exponentially in the $x \to \pm\infty$ limit, depending on the sign of $\mathrm{Im}(k)$. In what follows we study the various combinations of k and L.

Applying the $\mathcal{PT}$ operator on (9) and taking into consideration (2), (10) and the properties of the confluent hypergeometric function, the following relations are obtained:

$$\mathcal{PT}\Psi_q(x) = C_q^* \,\mathrm{e}^{k^*t(x)}(-t(x))^{\omega(q,L^*)} \times {}_1F_1(\omega(q,L^*) - \mathrm{i}Z/(2k^*), 2\omega(q,L^*), -2k^*t(x)) \tag{11}$$

$$= C_q^*(-1)^{\omega(q,L^*)}\,\mathrm{e}^{-k^*t(x)}(t(x))^{\omega(q,L^*)} \times {}_1F_1(\omega(q,L^*) + \mathrm{i}Z/(2k^*), 2\omega(q,L^*), 2k^*t(x)). \tag{12}$$

The latter equation follows from the properties of the confluent hypergeometric function [18].

2.2 *The case of real L*

For real values of $L = L^*$, eqs (11) and (12) turn into

$$\mathcal{PT}\Psi_q(x) = C_q^*(-1)^{\omega(q,L)}\,\mathrm{e}^{k^*t(x)}(t(x))^{\omega(q,L)} \times {}_1F_1(\omega(q,L) - \mathrm{i}Z/(2k^*), 2\omega(q,L), -2k^*t(x)) \tag{13}$$

$$= C_q^*(-1)^{\omega(q,L)}\,\mathrm{e}^{-k^*t(x)}(t(x))^{\omega(q,L)} \times {}_1F_1(\omega(q,L) + \mathrm{i}Z/(2k^*), 2\omega(q,L), 2k^*t(x)). \tag{14}$$

If k is real, i.e. $k^* = k$, then by comparing (9) and (14) it follows that the solutions (9) are eigenfunctions of the $\mathcal{PT}$ operator with unit eigenvalue if the phase of the normalization constant C_q is chosen as

$$C_q^* = \exp(\mathrm{i}\pi\omega(q,L)). \tag{15}$$

Applying the U-shaped trajectory proposed in ref. [11] and applied in ref. [12] the solutions exhibit oscillatory behaviour, and, at the same time the energy eigenvalue in (7) will be positive, due to $m < 0$. So this case corresponds to scattering solutions.

For imaginary values of k, i.e. $k^* = -k$ (13) again, reproduces (9) if the condition (15) holds. The solutions now become asymptotically regular due to the exponential factor $e^{k^* t(x)} \to e^{(-k_I^* |x|)}$ provided that $k_I = \mathrm{Im}(k) > 0$. The confluent hypergeometric functions also turn into generalized Laguerre polynomials [18] for $\omega(q, L) + iZ/(2k) = -N$, where N is a non-negative integer. Then from (7) it follows that

$$E_{n,q} = -\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 Z^2}{8m(n + \omega(q, L))^2} \tag{16}$$

which is negative due to $m < 0$ and recovers the known bound-state energy eigenvalues for $q = \pm 1$ [9]:

$$E_{n,+1} = \frac{\hbar^2 Z^2}{8m(n + L + 1)^2}, \quad E_{n,-1} = \frac{\hbar^2 Z^2}{8m(n - L)^2}. \tag{17}$$

Note that in ref. [9] the eigenvalues carried opposite sign.

2.3 *The case of* $L = -\frac{1}{2} + i\lambda$

In this case

$$\omega(q, L) = \frac{1}{2} + iq\lambda. \tag{18}$$

So

$$\omega(q, L^*) = \omega(-q, L) \tag{19}$$

holds. With this eqs (11) and (12) turn into

$$\begin{aligned} \mathcal{PT}\Psi_q(x) &= C_q^* \, e^{k^* t(x)} (-t(x))^{\omega(-q,L)} \\ &\quad \times {}_1F_1(\omega(-q, L) - iZ/(2k^*), 2\omega(-q, L), -2k^* t(x)) \qquad (20) \\ &= C_q^* (-1)^{\omega(-q,L)} \, e^{-k^* t(x)} (t(x))^{\omega(-q,L)} \\ &\quad \times {}_1F_1(\omega(-q, L) + iZ/(2k^*), 2\omega(-q, L), 2k^* t(x)). \qquad (21) \end{aligned}$$

Considering again the $k^* = k$ and $k^* = -k$ cases separately, eqs (20) and (21) lead to the same result, i.e. the $\mathcal{PT}$ operation transforms the two independent solutions into each other:

$$\mathcal{PT}\Psi_q(x) = \frac{C_q^*}{C_{-q}} (-1)^{\omega(-q,L)} \Psi_{-q}(x) = \exp(2\pi q\lambda) \frac{C_q}{C_{-q}} \Psi_{-q}(x), \tag{22}$$

where, in the second equation we made use of the phase convention (15). For $C_{+1} = \exp(-2\pi\lambda) C_{-1}$ the constant factors in (22) can be set to unity.

The $k^* = -k$ case, i.e. that of the discrete energy eigenvalues leads to interesting consequences regarding the energy eigenvalues. Substituting (18) in (16) the following discrete energy eigenvalues are obtained:

$$E_{n,q} = -\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 Z^2}{2m(2n+1+2\mathrm{i}q\lambda)^2} \ . \tag{23}$$

This means that not only will the wave functions cease to be the eigenfunctions of the $\mathcal{PT}$ operator, but at the same time, the energy eigenvalues turn into complex conjugate pairs which belong to the two possible values of the q quasi-parity quantum number. This is clearly the spontaneous breakdown of $\mathcal{PT}$ symmetry observed in many other $\mathcal{PT}$-symmetric potentials. The complexification of the energy spectrum typically happens when the coupling coefficient of the non-Hermitian potential component reaches a critical level. In the present case complex energy eigenvalues appear when $L(L+1) = -1/4 - \lambda^2$ gets below $-1/4$. Since in (3) both potential components are complex due to the complex trajectory $t(x)$, the separation of the real and imaginary potential components is not trivial. It is true, however, that increasing λ corresponds to increasing non-Hermiticity in the sense that the magnitude of the imaginary potential component increases. However, the same happens with that of the real potential component too.

3. Summary

With the present work we completed the study of various solutions of the $\mathcal{PT}$-symmetric Coulomb problem which we started in ref. [9] by deriving the bound-state solutions, continued with the re-interpretation of the problem along a U-shaped trajectory in the complex plane [11] and the calculation of the scattering solutions and the transmission and reflection coefficients along this path [12]. Here we focussed on discrete complex-energy solutions of the Coulomb potential, the appearance of which usually indicates the spontaneous breakdown of $\mathcal{PT}$ symmetry.

By a systematic study of various combinations of the L parameter and the wave numbers k (i.e. situations in which they are real or complex) we observed that for the $L = -\frac{1}{2} + \mathrm{i}\lambda$ case the potential maintains $\mathcal{PT}$ symmetry, but the energy spectrum turns complex and the two independent solutions distinguished by the quasi-parity quantum number are transformed into each other by the $\mathcal{PT}$ operator.

It is notable that although the parametrization (4) of the trajectory contains the ε parameter explicitly and ε appears in the wave functions too, the energy eigenvalues (17) and (23) are independent of it. This means that the energy eigenvalues do not change if curves with different ε are considered. The situation is similar to that encountered in the case of $\mathcal{PT}$-symmetric potentials defined in a line parallel to the x-axis in the complex plane as $x \to x + \mathrm{i}c$. In these studies [16,17] on the $\mathcal{PT}$-symmetric Scarf II and generalized Pöschl–Teller potentials it was found that although the wave functions depend on the parameter c, the energy eigenvalues do not. However, c also appeared in the transmission and reflection coefficients, typicaly in exponential forms. This also seems to be the case here, since in [12] it was also found that the transmission and reflection coefficients of the complex $\mathcal{PT}$-symmetric Coulomb potential also depend on ε in a similar way. It appears thus that the parameters setting the distance of the trajectory from the real or imaginary x-axis play a similar role in the two cases.

Although the necessity of defining the problem on a $\mathcal{PT}$-symmetric trajectory in the complex plane makes the present potential rather different from solvable

$\mathcal{PT}$-symmetric potentials defined on the real x-axis or on its imaginary shifted version $x - \mathrm{i}c$, the results obtained are in line with the characteristic features of these latter potentials. These features include the mechanism of the spontaneous breakdown of $\mathcal{PT}$-symmetry, i.e. all the energy eigenvalues turn into complex conjugate pairs at the same time; the appearance of the $q = \pm 1$ quasi-parity quantum number, which, for real energy eigenvalues distinguishes between the two sets of discrete solutions, while for complex energy eigenvalues it orders the complex conjugate energies into a pair. Together with the findings of ref. [12] on the transmission and reflection coefficients it is thus reasonable to claim that this unusual potential exhibits more similarities with more conventional $\mathcal{PT}$-symmetric potentials than differences.

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