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Asymptotically vanishing $\mathcal{PT}$-symmetric potentials and negative-mass Schrödinger equations

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ABSTRACT

In paper I [M. Znojil, G. Lévai, Phys. Lett. A 271 (2000) 327] we introduced the Coulomb–Kratzer bound-state problem in its crypto-Hermitian, $\mathcal{PT}$-symmetric version. An instability of the original model is revealed here. A necessary stabilization is achieved, for almost all couplings, by an unusual, negative choice of the bare mass in Schrödinger equation.

1. Introduction

Intuitively one feels that for Schrödinger equations

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

there should exist a close connection between the reality of potential $V(x)$ and the reality of the corresponding energies E. Unfortunately, such a type of intuition proves deceptive. Recent studies (e.g., [1] or [2]) showed that many manifestly non-Hermitian potentials, e.g.,

$$V^{(BB)}(x)=x^2(\mathrm{i}x)^{4\delta},\quad \delta\geqslant 0, \tag{2}$$

still lead to a full reality of the spectrum. The key to such an unexpected phenomenon can be seen in the Bender's and Boettcher's [1] fortunate choice of a complex integration contour $x=x^{(BB)}(s)$ in Eq. (1). Its asymptotes

$$x^{(BB)}(s)\approx\begin{cases} se^{\mathrm{i}\varphi}, & s\gg 1,\\ se^{-\mathrm{i}\varphi}, & s\ll -1\end{cases}, \tag{3}$$

were restricted to the δ-dependent interval of angles,

$$\varphi+\frac{\pi}{2}\in\left(\frac{\pi}{4+4\delta},\frac{3\pi}{4+4\delta}\right). \tag{4}$$

The curve itself was required not to cross the singularity of $V^{(BB)}(x)$ in the origin, $\mathrm{i}x^{(BB)}(0)>0$. In this setting one can impose the standard Dirichlet boundary conditions at the ends of the left–right-symmetric curve of complex coordinates, $\Psi(x^{(BB)}(\pm\infty))=0$, with the computationally preferred slope lying precisely in the center of the interval,

$$\varphi^{(BB)}=\frac{\pi}{2+2\delta}-\frac{\pi}{2}. \tag{5}$$

In Ref. [1] it has been emphasized that potentials (2) as well as paths of x and angles (5) were chosen as symmetric with respect to the combination of the parity-reversal symmetry mediated by the operator $\mathcal{P}$ with the time-reversal symmetry represented by operator $\mathcal{T}$ (cf. also Ref. [3] in this respect). In Ref. [4] it has been added that for the other eligible domains of angles, say, for

$$\varphi+\frac{\pi}{2}\in\left(\frac{3\pi}{4+4\delta},\frac{5\pi}{4+4\delta}\right) \tag{6}$$

the reality of the spectrum breaks down at some non-vanishing exponents $\delta<\delta_0$. In this sense the specific $\mathcal{PT}$-symmetric choice of (2)–(4) giving $\delta_0=0$ may be considered optimal.

The discussions in Refs. [1,4] did not involve the negative exponents δ and, in particular, the short-range models where $V(\infty)=0$. The gap has partially been filled by Ref. [5] where we studied Eq. (1) with one of the simplest possible asymptotically vanishing $\mathcal{PT}$-symmetric potentials of the Coulomb–Kratzer two-parametric form,

$$V(x)=V^{(CK)}(x)=\frac{\mathrm{i}Z}{x}+\frac{F}{x^2}. \tag{7}$$

This model admits $\varphi\in(0,\pi)$ (cf. Eq. (4) with $2\delta=-1$). From Eq. (5) giving $\varphi^{(BB)}=\pi/2$ one arrives at the U-shaped complex-coordinate contours $x^{(BB)}(s)$ as sampled in Fig. 1 where the cut is assumed from $x=0$ upwards. Marginally let us emphasize that our Schrödinger equation (1) in the most common physical setting using an integer angular momentum $\ell=0,1,\dots$ should in fact be considered with the "centrifugal-like" term of a non-integer strength $L(L+1)=\ell(\ell+1)+F$ in general.

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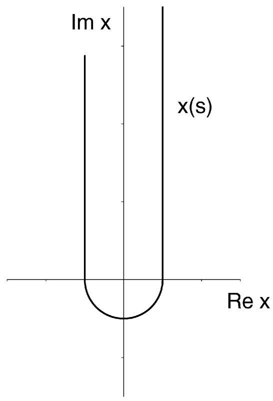

Fig. 1. The optimal, U-shaped contour of the complexified coordinates $x^{(\mathrm{BB})}(s)$ for the Coulomb–Kratzer $\mathcal{PT}$-symmetric potential (7).

At the time of the publication of Ref. [5] (to be cited as paper I from now on) the physical meaning of the similar models remained still rather obscure. Many authors studied and interpreted them as mere effective non-Hermitian simulations of spectra, not allowing any immediate physical interpretation of the related wave functions $\Psi(x) \in \mathbb{L}_2(\mathbb{R})$. Although we also accepted the same philosophy in paper I, we were aware of the fact that such an attitude significantly weakened the impact and practical applicability of similar studies.

Fortunately, the subsequent development of the subject clarified that the potentials as exemplified by Eq. (7) can be interpreted as fully compatible with the standard postulates and probabilistic interpretation of Quantum Mechanics. One of the most straightforward *mathematical* keys to the resolution of such an apparent puzzle can be seen in the existence of a suitable *non-unitary* invertible map Ω between some manifestly non-Hermitian Hamiltonians $H \neq H^\dagger$ and their manifestly Hermitian partners $\mathfrak{h} = \Omega H \Omega^{-1}$ (cf., e.g., Ref. [6] for a compact explanation of this mathematical idea).

From the point of view of physics, the historical origin of the idea of relevance of isospectrality between $\mathfrak{h}$ and H can be traced back to the study of models of atomic nuclei [7]. There an explicit example of operator $\Omega \neq (\Omega^\dagger)^{-1}$ has been provided by the generalized Dyson mappings [8]. Our recent return to these physical studies in our mathematical review [6] showed that for the $\mathcal{PT}$-symmetric models all the probabilistic physical postulates of quantum theory remain valid.

Among immediate and most recent phenomenological applications of non-Hermitian, $\mathcal{PT}$-symmetric operators $H \neq H^\dagger$ with real spectra let us mention here just the preprint [9] dealing with a $\mathcal{PT}$-symmetric version of a flat Friedmann model in quantum cosmology. In such a broader physical context we feel particularly inspired here by one of technical questions discussed in this Letter and concerning the possible instabilities of generic $\mathcal{PT}$-symmetric systems. In this sense we also returned to our older results of paper I which will be re-evaluated, corrected and re-interpreted in what follows.

2. Free motion along asymptotes

In the majority of presentations of Schrödinger equation (1) in textbooks one works with the real x specifying the position of a particle or quasiparticle which carries a constant mass $m = m_0 > 0$. The influence of external forces is modeled solely by a potential $V(x)$. During the last few years a manifest coordinate-dependence of the mass term has been allowed as well [10]. The choice of $m = m(x)$ opened new perspectives in an optimal description of the effects of medium.

This idea could easily be transferred to the present class of models where $x = x(s)$ is complex and where the effect of the potential becomes negligible in the asymptotic domain of $|s| \gg 1$. In such a setting the mass can be perceived as a potentially position-dependent *complex* quantity, $m = m[x(s)] \in \mathbb{C}$.

At the large $|s|$ our Hamiltonians get approximated by the kinetic-energy operator T which, by itself, gets complexified in the light of Eq. (3),

$$T = -\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2} = \begin{cases} -e^{-2i\varphi}\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2}, & s \gg 1, \\ -e^{+2i\varphi}\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2}, & s \ll -1. \end{cases} \tag{8}$$

Once we introduce the asymptotically constant complex effective local mass $m_{\mathrm{eff}}[x(s)]$ it will only depend on the slope φ and on the sign of s,

$$T = -\frac{\hbar^2}{2m_{\mathrm{eff}}}\frac{d^2}{ds^2}, \quad m_{\mathrm{eff}} = m_{\mathrm{eff}}\big[x(s)\big] = \begin{cases} e^{2i\varphi}m_0, & s \gg 1, \\ e^{-2i\varphi}m_0, & s \ll -1. \end{cases} \tag{9}$$

This observation is too abstract, for several reasons. First of all, a subtle balance between the left and right branches of wave functions $\Psi[x(s)]$ exists and reestablishes the reality of the energies for numerous complex interactions $V[x(s)]$ [11]. Secondly, for $m = m(x)$ the well-known von Roos' [10] ambiguity of the kinetic energy would emerge at the finite values of s. For complex $x(s)$ the manifest introduction of the coordinate-dependence in the mass might also lead to many other technical complications. For these reasons our present attention will solely be paid to the models where m_{eff} remains constant. Using just the asymptotically vanishing potentials exemplified by Eq. (7) and assuming the local reality of the kinetic energy we shall only make a choice between $\varphi = 0$ and $\varphi = \pi/2$. In this way we encounter either the entirely traditional textbook straight-line models at $\varphi = 0$ or their U-shaped-line innovations at $\varphi = \pi/2$.

As long as the former case is very traditional let us only discuss the choice of $\varphi = \pi/2$ giving the U-shaped contours sampled in Fig. 1. Since *both* their asymptotes parallel the *upper* imaginary half-axis (i.e., a cut from $x = 0$ upwards), the phase of the complex numbers will be assumed lying in the interval $(-3\pi/2, \pi/2)$. Under such a convention and in terms of a suitable width parameter $\varepsilon > 0$ we may parametrize the contours of Fig. 1 as follows,

$$x(s) = x^{(U)}_{(\varepsilon)}(s) = \begin{cases} -i(s + \frac{\pi}{2}\varepsilon) - \varepsilon, & s \in (-\infty, -\frac{\pi}{2}\varepsilon), \\ \varepsilon e^{i(s/\varepsilon - 1/2\pi)}, & s \in (-\frac{\pi}{2}\varepsilon, \frac{\pi}{2}\varepsilon), \\ i(s - \frac{\pi}{2}\varepsilon) + \varepsilon, & s \in (\frac{\pi}{2}\varepsilon, \infty). \end{cases} \tag{10}$$

In the complex plane of x the latter curve exhibits the double-reflection left–right symmetry $x(-s) = -x^*(s)$ which combines the spatial reflection $\mathcal{P}$ with the complex conjugation $\mathcal{T}$ (let us recollect that $\mathcal{T}: i \to -i$ mimics time-reversal). Fig. 2 shows how such a curve of the complex coordinates could be deformed in the limit $\varepsilon = 0$. It still encircles the origin at a distance but its asymptotes already strictly coincide with the upper imaginary half-axis.

Let us emphasize that for $\varphi = \pi/2$ the coordinate-independence of the effective mass simplifies the kinetic-energy operator

$$T = -\frac{\hbar^2}{2m_0}\frac{d^2}{dx^2} = +\frac{\hbar^2}{2m_0}\frac{d^2}{ds^2} \quad \text{at } |s| \gg 1. \tag{11}$$

Surprisingly enough, it acquires the wrong sign in the sense that its spectrum becomes unbounded from below at the positive "bare mass" $m_0 > 0$. This would make the whole system unstable with respect to small perturbations and, hence, useless for any phenomenological purposes.

There are hints that also in a field theoretical framework similar considerations hold concerning negative kinetic energy encountered during quantization of classical phantom Lagrangians [9]. This encourages us to make our argument more quantitative. Let us