Exact solution for Morse oscillator
in $\mathcal{PT}$–symmetric quantum mechanics

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Abstract

$\mathcal{PT}$ invariance of complex potentials $V(x) = [V(-x)]^*$ combines their real symmetry with imaginary antisymmetry. We describe a new exactly solvable model of this type. Its spectrum proves real, discrete and “three-fold”, $\varepsilon = \varepsilon_n(j) = (2n + \alpha_j)^2$, $n = 0, 1, \ldots$, with $\alpha_j \geq 0$ and $j = 1, 2, 3$.

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Recently, Daniel Bessis [1] and Bender and Boettcher [2] proposed a certain modification of the interpretation of the one-dimensional Schrödinger-like differential equations. In a way inspired by the methodical relevance of the spatially symmetric harmonic oscillator in field theory [3] they tried to weaken the standard assumption of hermiticity of the Hamiltonian $H = H^+$, i.e., in the strict mathematical language, the requirement of the essentially self-adjoint character of this operator.

The new idea has found its first physical applications and immediate tests in field theory (cf., e.g., refs. [4] for explicit illustrations). Its use in the time-independent quantum mechanics has simultaneously been proposed [5]. As long as the time-reversal operator $T$ performs the mere Hermitian conjugation in the latter case, a generalization of bound states with definite parity ($\mathcal{P}\psi = \pm \psi \in L_2$) has been found in normalizable states with a parity-plus-time-reversal combined symmetry ($\mathcal{P}\mathcal{T}\psi = \pm \psi \in L_2$).

In the $\mathcal{PT}$-symmetric quantum mechanics a stability hypothesis $\text{Im} \, E = 0$ has been tested semi-classically [2, 3], numerically [1, 6], analytically [7, 8] and perturbatively [9, 10]. One may even return to the related older literature, say, on the cubic anharmonic oscillator $V(x) = \omega^2 + igx^3$, all the resonant energies of which remain real and safely bounded below [9, 11]. The similar complete suppression of decay has now been observed and/or proved in several other analytic models [12, 13].

Serious problems arise for the non-analytic $\mathcal{PT}$-symmetric interactions [5]. An indirect clarification of the difficulty is being sought, first of all, in the various analytic $\mathcal{PT}$-analogs of the usual square well [8, 9, 14]. In the present note, another exactly solvable example of such a type will be proposed and analyzed in detail, therefore.

Let us start by characterizing solvable potentials by their so called shape invariance. The review [15] lists nine of these models. Once we restrict our attention to the mere confluent-hypergeometric-type equations on full line, we are left with the spatially symmetric harmonic oscillator $V^{(\text{HO})}(r) = \omega^2 (r - b/\omega)^2 - \omega$ and with its Morse-oscillator partner

$$V^{(\text{Morse})}(r) = A^2 + B^2 \exp(-2\beta r) - 2B(A - \beta/2) \exp(-\beta r).$$  (1)
The \( \mathcal{PT} \)–symmetrization of the former model \( V^{(HO)} \) has been recalled in the pioneering paper [2]. The latter case \( (\Pi) \) is to be considered here.

The real and Hermitian version of the model \( V^{(Morse)} \) is of a non-ceasing interest in the current literature [16]. Its consequent \( \mathcal{PT} \)–symmetrization necessitates a few preliminary considerations. In the first step, let us make a detour and return once more to the real and Hermitian \( V^{(HO)} \) and to its generalized three-dimensional Schrödinger-equation presentation

\[
\left[ -\frac{d^2}{dr^2} + \omega^2 r^2 + \frac{\ell (\ell + 1)}{r^2} \right] \psi(r) = E\psi(r), \quad \ell = -\frac{1}{2} + \alpha, \ \alpha > 0. \quad (2)
\]

We may remind the reader that one can safely return back by choosing the trivial \( \ell = -1 \) and/or \( \ell = 0 \). Still, beyond this special “full-line” case with parity \( (-1)^{\ell+1} \), the singularity at \( r = 0 \) remains prohibitively strong for any \( \alpha > 0 \).

Fortunately, according to our recent letter [17], an unexpected remedy may be found in the \( \mathcal{PT} \)–symmetrization. It renders even the singular equation (2) tractable on the full line. The core of its \( \mathcal{PT} \)–regularization lies in an analytic continuation in the coordinate \( r \). This enables us to work in the complex plane with an appropriately chosen cut. The cut starts at the singularity in \( r = 0 \) and may be directed, conveniently, upwards. In such a setting one may integrate equation (2) along the real line which is only slightly shifted downwards. In the notation with \( r = s - ic, \ c > 0 \) and with a new real quasi-coordinate \( s \in (-\infty, \infty) \) the physical boundary conditions \( \psi(-ic \pm \infty) = 0 \) remain the same as before.

A non-numerical key to the complexified one-dimensional problem (2) lies in a surviving exhaustive solvability of its differential equation in terms of the confluent hypergeometric functions,

\[
e^{\omega r^2 / 2} \psi(x) = C_1 r^{-\alpha + 1/2} {}_1F_1 \left( (2 - 2\alpha - E/\omega)/4, 1 - \alpha; \omega r^2 \right) + \]

\[
+ C_2 r^{\alpha + 1/2} {}_1F_1 \left( (2 + 2\alpha - E/\omega)/4, 1 + \alpha; \omega r^2 \right). \quad (3)
\]

For the large coordinates \( r \) which lie within the wedges \(|\text{Im} r| < |\text{Re} r|\), both these hypergeometric series grow as \( \exp(\omega r^2 / 2) \) or, alternatively, degenerate to a polynomial [18]. Discarding the former possibility as manifestly violating our physical
boundary conditions we arrive at a slightly unusual formula for the binding energies

\[ E = E_{qn} = \omega(4n + 2 - 2q\alpha), \quad q = \pm 1, \quad n = 0, 1, 2, \ldots \]

and get also wave functions containing Laguerre polynomials,

\[ \psi(r) = \text{const.} r^{-q\alpha+1/2} e^{-\omega r^2/2} L_n^{(-q\alpha)} \left( \omega r^2 \right). \]

The spectrum remains real, discrete and bounded below and it reproduces the current, equidistant harmonic energies at \( \alpha = 1/2 \) \(^7\).

A change of the coordinates \( r = \text{const} \times \exp(\text{const} \, x) \) mediates a transition to the Morse forces \( V^{Morse} \). We have to convert the asymptotically normalizable harmonic wavefunctions \( \psi_{n,\pm}(r) \sim \exp(-\omega r^2/2), \ Re \, r \to \pm \infty \) to their Morse asymptotically normalizable counterparts \( \varphi(x) \). Using the explicit rule

\[ r = -i e^{ix}, \quad \psi(r) = \sqrt{r} \varphi(x) \quad (4) \]

in the harmonic Schrödinger equation (2) we arrive at the \( \mathcal{PT} \)–symmetrized Morse bound-state problem

\[ \left[ -\frac{d^2}{dx^2} - \omega^2 \exp(4ix) - D \exp(2ix) \right] \varphi(x) = \varepsilon \varphi(x). \quad (5) \]

Our change of variables maps the straight integration contour \( r = s - \text{i}c \) with the real \( s \in (-\infty, \infty) \) and with the positive constant \( c > 0 \) onto the deformed, down-bent curve

\[ \mathcal{C} = \{ x = v - iu \mid v \in (-\pi/2, \pi/2), \ u = u(v) = \ln(c/\cos v) \}. \quad (6) \]

The circles centered at the origin are mapped upon segments of horizontal lines. The upward-running cut from \( r = 0 \) to \( r = i\infty \) is represented, due to the periodicity of the exponential, by an infinite family of the vertical lines. The whole plane of \( r \) is mapped on the single vertical strip in \( x \), and the multi-sheeted Riemann surface in \( r \) is projected upon the whole complex \( x \)--plane.

Our manifestly \( \mathcal{PT} \) symmetric equation (3) contains the Morse potential (1) where \( \beta = -2i, \ B = i\omega \) and \( A = i(1 - E/2\omega) \). The old energy \( E \) is to be re-interpreted as a new coupling \( D = E \). The old centrifugal-like parameter \( \alpha = \ell + 1/2 \)
re-appears as a new momentum and specifies the Morse energy $\epsilon = \alpha^2$. The original harmonic oscillator recipe $\alpha \to E_n$ is replaced by the new equivalent rule $D \to \alpha_m^2$. This is because the new integration contour $C$ preserves the asymptotic growth or decrease of the general solutions (3).

At first sight, the latter conclusion may seem slightly confusing. Its clarification is easy. In equation (3) the real parameters $v$ and $u$ are such that the values of $v$ remain bounded. The variation of $v$ parameterizes not only $s = c \tan v$ but also both the two semi-infinite branches of $u(v) \in (\ln c, \infty)$. By construction, the harmonic-oscillator states with the even and odd quasi-parity $q = \pm 1$ and energies $E = E_{n,\pm 1}(\alpha) = \omega(4n + 2 \mp 2\alpha)$, $n = 0, 1, \ldots$ are mapped upon the new Morse bound states with the energies

$$\epsilon = \epsilon_m^{[\mp]}(D) = (2m + 1 \mp D/2\omega)^2, \quad m = 0, 1, \ldots.$$  \hspace{1cm} (7)

*Mutatis mutandis*, also the wave functions are easily obtained. One only has to pay attention to the unavoided $[17]$ crossings at the integers $D/2\omega$.

Phenomenologically, the new spectrum is fairly rich. For $D/4\omega = M + \sigma - 1/2 > 0$ with a small $\sigma \in (0, 1)$ and an appropriate integer $M \geq 0$ the set of the quasi-even energies splits in the two subsequences. The first one is finite,

$$\epsilon_{M-k-1}^{[+]}(D)/4 = (k + \sigma)^2, \quad k = 0, 1, \ldots, M - 1 \hspace{1cm} (8)$$

and decreases with the number of nodes in $\varphi(x)$. The infinite rest is increasing,

$$\epsilon_{M+k}^{[+]}(D)/4 = (k + 1 - \sigma)^2, \quad k = 0, 1, \ldots \hspace{1cm} (9)$$

In contrast, all the quasi-odd energies exhibit a monotonic growth and remain minorized by a positive constant $(D/2\omega + 1)^2/4$,

$$\epsilon_k^{-}(D)/4 = (k + M + \sigma)^2, \quad k = 0, 1, \ldots, \hspace{1cm} (10)$$

This split of the spectrum into its three sub-families (8) + (9) + (10) is illustrated in Table [1], which samples re-orderings of the energy levels in dependence on the growth of the coupling $D$. Once we ignore the superscripted quasi-parities (and, perhaps, a
possible separation of the ground state) the spectrum may be visualised as an infinite sequence of doublets \((\varepsilon_k, \varepsilon_l)\). Their square roots are in fact equidistant.

We may summarize that our \(\mathcal{PT}\)–symmetrized Morse model \(^5\) is completely characterized by its mapping \(^6\) on the singular harmonic oscillator. One only has to note that the mapping need not be invertible easily. Indeed, in the complex \(x\)–plane, our HO-inspired integration contour \(\mathcal{C} = \mathcal{C}(-1,1)\) is by far not unique. Firstly, due to the absence of singularities in eq. \(^7\) the non-asymptotic parts of its curved integration contour \(\mathcal{C}\) may be further deformed. One only has to leave the asymptotics of \(\mathcal{C}\) unchanged. Secondly, an asymptotically different curve \(\mathcal{C}(-k,l)\) of ref. \(^8\) may be chosen as well \(^9\). It is characterized by the two odd integers \(k\) and \(l\) and formed by the respective left and right branches \(x = v - iu\) with \(u = \ln(c/\cos v)\) and \(v \in (-k\pi/2, -(k-1)\pi/2) \cup ((l-1)\pi/2, l\pi/2)\), pasted together by a (say, straight) line with \(v \in (- (k - 1) \pi/2, (l - 1) \pi/2)\).

The feasibility of the non-numerical implementation of the latter idea remains an open question. Formally, the new, more general Morse-Schrödinger differential equation remains \(\mathcal{PT}\) invariant and the manifest \(\mathcal{PT}\) symmetry is also exhibited by its boundary conditions. In principle, the new spectrum of energies should remain real and bounded below. In practice, the proof must be delivered independently. Via a backward mapping, the modified system would be equivalent to a generalized harmonic oscillator with the nontrivial integration curve encircling the essential singularity in the origin and moving (perhaps, repeatedly, through the cut) to the second (or other) Riemannian sheet(s).

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Table 1: The $D$–dependence and pairing of the low-lying spectra (7). The level-crossings occur precisely at the even ratios $D/4\omega$. The energy doublets remain formed in their vicinity. The equidistance of the moments $\sqrt{\epsilon_n^\pm}(D)$ only takes place at the odd integers $D/4\omega$.

| $D/4\omega$ | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | … |
|-------------|-----|-----|-----|-----|-----|-----|-----|-----|----|
| $\epsilon_3^+$ | $\epsilon_3^+$ | $\epsilon_2^-$ | $\epsilon_2^-$ | $\epsilon_4^+$ | $\epsilon_4^+$ | $\epsilon_1^-$ | $\epsilon_1^-$ | $\epsilon_5^+$ | … |
| $\epsilon_2^+$ | $\epsilon_2^+$ | $\epsilon_1^-$ | $\epsilon_1^-$ | $\epsilon_3^+$ | $\epsilon_3^+$ | $\epsilon_0^-$ | $\epsilon_0^-$ | $\epsilon_4^+$ | … |
| $\epsilon_2^+$ | $\epsilon_1^-$ | $\epsilon_1^-$ | $\epsilon_3^+$ | $\epsilon_3^+$ | $\epsilon_0^-$ | $\epsilon_0^-$ | $\epsilon_4^+$ | $\epsilon_0^+$ | $\epsilon_0^+$ |
| $\epsilon_1^+$ | $\epsilon_1^+$ | $\epsilon_0^-$ | $\epsilon_0^-$ | $\epsilon_2^+$ | $\epsilon_2^+$ | $\epsilon_0^+$ | $\epsilon_0^+$ | $\epsilon_3^+$ | $\epsilon_3^+$ |
| $\epsilon_0^-$ | $\epsilon_0^-$ | $\epsilon_1^+$ | $\epsilon_1^+$ | $\epsilon_0^+$ | $\epsilon_0^+$ | $\epsilon_2^+$ | $\epsilon_2^+$ | $\epsilon_1^+$ | $\epsilon_1^+$ |