Pöschl–Teller paradoxes

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Abstract
In the well-known Pöschl–Teller trigonometric potential well, a $\mathcal{PT}$-symmetric
regularization $x \to x - \mathrm{i}\,\varepsilon$ of the 'impenetrable' end-point barriers is performed.
This leads to the four different solvable generalizations of the model. As a
byproduct, the scheme clarifies certain apparent paradoxes encountered in the
classically forbidden coupling regime.

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1. Introduction

The Pöschl–Teller [1] potential

$$V^{(A,B)}(x) = \frac{A(A-1)}{\cos^2 x} + \frac{B(B-1)}{\sin^2 x} \tag{1}$$

may be visualized as a sequence of asymmetric wells separated by impenetrable barriers
(cf figure 1 where $t = 2x/\pi$ and we choose $A = 2.5$ and $B = 1.25$). Each of these wells (say,
the one defined on the interval $x \in (0, \pi/2)$) admits the fully non-numerical treatment. The
review paper [2] lists its bound-state spectrum

$$E_n = (A + B + 2n)^2 \qquad n = 0, 1, \dots \tag{2}$$

(its three lowest levels are also indicated in figure 1) as well as the corresponding wavefunctions
which are proportional to the Jacobi polynomials,

$$\psi_n(x) = \cos^A x \cdot \sin^B x \cdot P_n^{(B-1/2, A-1/2)}(\cos 2x). \tag{3}$$

It is concluded that '*the requirement of $A, B > 0 \dots$ guarantees*' that each wavefunction
ψ_n in equation (3), '*is well behaved and hence acceptable as $x \to 0, \pi/2$*' [2, p 295].
Obviously, the quantized system remains stable even in the classically collapsing regime with
$A(A-1) \in (-1/4, 0)$ (a (weak) barrier reoriented downwards at the right end ($x = \pi/2$)) or
$B(B-1) \in (-1/4, 0)$ (same at the left end ($x = 0$)). This is the well-known paradox [3, 4].

At $A = B$ we discover another one. The simplified potential does not change its shape and
only its strength varies with B, namely, $V^{(B,B)}(x) = g(B)/\sin^2 2x$, where $g(B) = 4B(B-1)$.
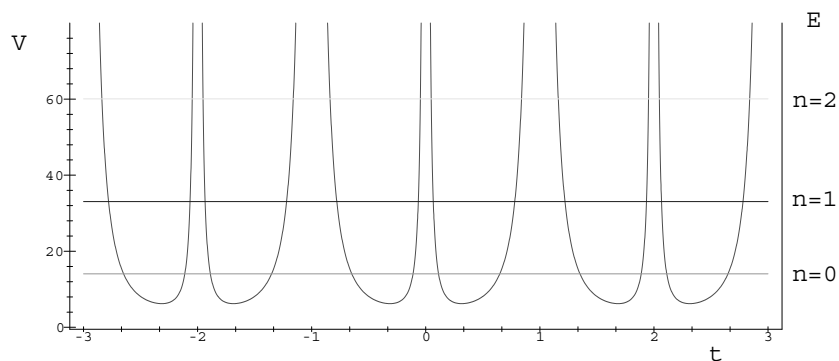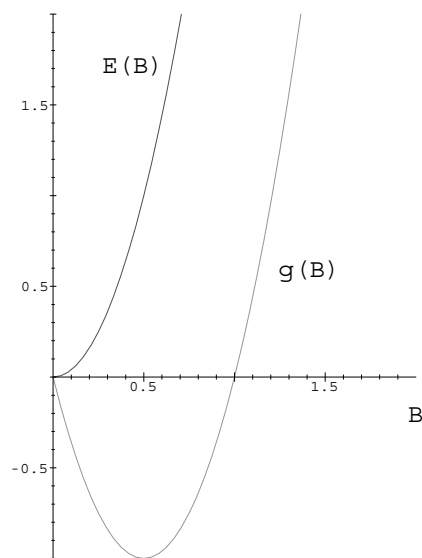
Figure 1. The Pöschl–Teller potential.

Figure 2. The paradox of review [2].

The ground state is formed at the energy $E_0 = 4B^2 = E(B)$. Nevertheless, at the smallest positive $B < 1/2$ the potential well moves down while, at the same time, the ground-state energy grows. This contradicts common sense and represents another paradox (cf figure 2).

An explanation of the latter puzzle is still elementary. It is sufficient to stay near $x = 0$ and imagine that the differential Schrödinger equation possesses the elementary general solution

$$\psi(x) \sim C_1 \, x^B + C_2 \, x^{1-B} \qquad x \approx 0. \tag{4}$$

In accordance with the textbooks, we will witness the collapse of the system (i.e. its unstoppable fall in the singularity $\mathcal{O}(x^{-2})$) when $\mathrm{Re}\, B = 1 - \mathrm{Re}\, B$ (i.e. at the point $B = 1/2$). It is necessary to require that $B > 1/2$. This means that the domain of $B \in (1/2, 1)$ has been counted twice in figure 2. The corrected B-dependence is displayed in figure 3. The decrease and growth of the energy $E_0 = E(B)$ merely reflect the underlying downward and upward movement of the potential. Unfortunately, the whole picture is not entirely satisfactory, at least for several purely psychological reasons:
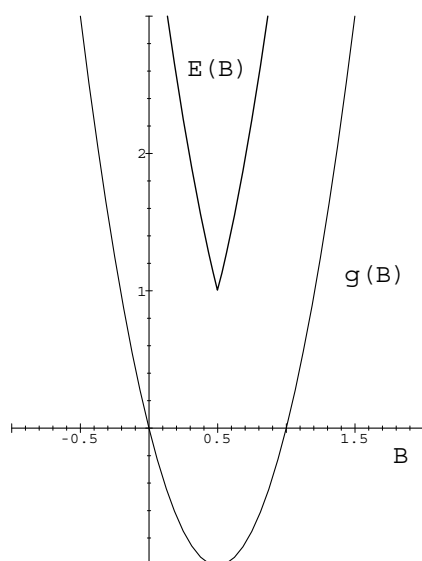
Figure 3. The corrected picture.

- The broken shape of the energy curve in figure 3 is counterintuitive.
- Although our duty of discarding the well-behaved solutions as unphysical can find many different mathematical explanations, it also goes against our basic instincts [5].
- People often search for psychologically persuasive explanations. One of the best arguments of the latter type applies, unfortunately, to the mere *regular s*-wave potentials [6].
- A fairly popular use of the various *ad hoc* conditions can make the appropriate quantization recipe quite enigmatic [7]. The subtleties of its implementation are often forgotten in quantum chemistry or atomic physics where strongly singular phenomenological models frequently occur [8, 9].

Therefore in what follows, we intend to offer a new, unusual approach to the Pöschl–Teller problem.

2. Complexification

In a purely intuitive setting our problem resembles the study of the elementary algebraic equation $x^2 + 2bx + c = 0$, where an irregularity appears along a parabola $c = c_{\text{crit}}(b) = b^2$. Outside this curve in the real (b, c) plane we always find the two real roots $x_{1,2} = -b \pm \sqrt{b^2 - c}$. Inside the curve, both of them suddenly disappear into the complex plane of x.

We shall treat the Pöschl–Teller paradoxes in a manner guided by this analogy.

2.1. $\mathcal{PT}$-symmetric picture

In essence, the proposal we are going to describe will replace the previous pictures by a new figure 4. Its mathematics will offer us the two smooth auxiliary curves $E^{(\pm)}(B)$. Their user will be permitted to make a choice between these two alternatives, employing in addition purely physical arguments and/or preferences.
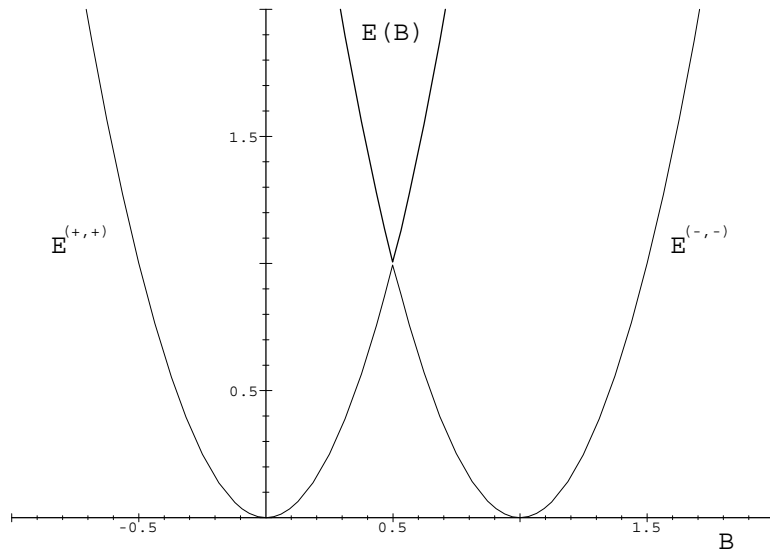
Figure 4. $\mathcal{PT}$-symmetric reinterpretation of figure 3.

The core of our proposal will lie in a certain complexification of the Pöschl–Teller differential Schrödinger equation in units of $2m = \hbar = 1$,

$$\left(-\frac{d^2}{dx^2} + \frac{\alpha^2 - 1/4}{\cos^2 x} + \frac{\beta^2 - 1/4}{\sin^2 x}\right)\psi(x) = E\,\psi(x) \qquad x \in \left(0, \frac{\pi}{2}\right) \qquad (5)$$

with $\alpha = A - 1/2 > 0$ and $\beta = B - 1/2 > 0$. We are inspired by the recent paper by Bender and Boettcher [10] who replace the real (interval of) coordinates x by a suitable complex curve $\mathcal{C}(t)$. On the basis of an extensive computational and WKB-based experience with many resulting non-Hermitian Hamiltonians, they conjecture that under certain weak conditions the spectrum can still stay real. In the present context, the most natural implementation of the latter idea is based on the elementary choice of the straight line

$$x \to \mathcal{C}(t) = x(t) = t - \mathrm{i}\,\varepsilon \qquad t \in (-\infty, \infty). \qquad (6)$$

It has been shown to work, e.g., for shape-invariant models [11] and for the whole Natanzon class of exactly solvable potentials [12].

One can easily observe that the curve (6) remains unchanged under the combined action of the parity $\mathcal{P}$ and of the 'time-reversal' (in fact, complex-conjugation) operator $\mathcal{T}$. One can speak about the specific, $\mathcal{PT}$-symmetric quantum mechanics [13]. Under certain mathematical assumptions and at least in a certain domain of couplings (both specifications are, by far, not yet clear [14]), one can often discover that the spectrum after deformation $x \to \mathcal{C}(t)$ remains discrete, bounded from below and *real* [15].

2.2. Wavefunctions

In a manner guided by the original paper by Pöschel and Teller [1], let us move to the complex x, abbreviate $\sin^2 x = y$, denote $\psi[x(y)] = \varphi(y)$ and rewrite our equation (5) using these new variables

$$y(1 - y)\,\varphi''(y) + \left(\frac{1}{2} - y\right)\varphi'(y) + \frac{1}{4}\left(E - \frac{\beta^2 - 1/4}{y} - \frac{\alpha^2 - 1/4}{1 - y}\right)\varphi(y) = 0. \qquad (7)$$

The ansatz $E = k^2$ and

$$\varphi(y) = y^\mu (1 - y)^\nu \, f(y)$$

transform our complexified differential equation in its Gauss hypergeometric equivalent

$$y(1 - y) f''(y) + \left[(2\mu + \tfrac{1}{2}) - (2\mu + 2\nu + 1) \, y \right] f'(y) + \left[\tfrac{1}{4} k^2 - (\mu + \nu)^2 \right] f(y) = 0$$

provided only that we choose μ and ν in accordance with the conditions

$$4\mu(\mu - 1) = \beta^2 - \tfrac{1}{4} \qquad 4\nu(\nu - 1) = \alpha^2 - \tfrac{1}{4}.$$

In terms of the two indeterminate signs these quadratic equations define two pairs of the eligible exponents,

$$2\mu = \tfrac{1}{2} + \sigma\beta = \kappa(\sigma) \qquad 2\nu = \tfrac{1}{2} + \tau\alpha = \lambda(\tau) \quad \sigma, \tau = \pm 1.$$

A general solution of our equation (5) acquires the τ-dependent compact form

$$\psi(x) = \left\{ C_1 \, \chi^{(\sigma,\tau)} [y(x)] \, \sin^{\kappa(\sigma)} x + C_2 \, \chi^{(-\sigma,\tau)} [y(x)] \, \sin^{\kappa(-\sigma)} x \right\} \cdot \cos^{\lambda(\tau)} x. \tag{8}$$

Here we have abbreviated

$$\chi^{(\sigma,\tau)}(y) = {}_2F_1 \left\{ \tfrac{1}{2} [\kappa(\sigma) + \lambda(\tau) + k], \tfrac{1}{2} [\kappa(\sigma) + \lambda(\tau) - k], \tfrac{1}{2} + \kappa(\sigma); y \right\}. \tag{9}$$

In an alternative representation, using the *same* constants C_1 and C_2 we have

$$\chi^{(\sigma,\tau)} [y(x)] \cdot \cos^{\lambda(\tau)} x = \varrho^{(\sigma,\tau)} [y(x)] \cdot \cos^{\lambda(\tau)} x + \varrho^{(\sigma,-\tau)} [y(x)] \cdot \cos^{\lambda(-\tau)} x \tag{10}$$

where

$$\varrho^{(\sigma,\tau)}(y) = G^{(\sigma,\tau)} \, {}_2F_1 \left\{ \tfrac{1}{2} [\kappa(\sigma) + \lambda(\tau) + k], \tfrac{1}{2} [\kappa(\sigma) + \lambda(\tau) - k], \tfrac{1}{2} + \lambda(\tau); 1 - y \right\} \tag{11}$$

with the factor

$$G^{(\sigma,\tau)} = \frac{\Gamma(1 + \sigma\beta) \, \Gamma(-\tau\alpha)}{\Gamma[\kappa(\sigma) + \lambda(-\tau) + k] \, \Gamma[\kappa(\sigma) + \lambda(-\tau) - k]} \, .$$

One of the immediate consequences of these two alternative expansions is our explicit knowledge of the related $0 < x \ll 1$ left-threshold leading-order approximation

$$x^{-1/2} \psi(x) \sim C_1 \, x^{\sigma\beta} + C_2 \, x^{-\sigma\beta} \tag{12}$$

and of its $0 < z = \pi/2 - x \ll 1$ right-threshold counterpart

$$z^{-1/2} \psi[x(z)] \sim \tilde{C}^{(+)} z^{\tau\alpha} + \tilde{C}^{(-)} z^{-\tau\alpha} \qquad \tilde{C}^{(\pm)} = \left[C_1 \, G^{(\sigma,\pm\tau)} + C_2 \, G^{(-\sigma,\pm\tau)} \right]. \tag{13}$$

We summarize that the complete solution of the Pöschl–Teller differential Schrödinger equation is available in a closed form even on any generalized, complex domain $\mathcal{C}$ of coordinates x characterized, presumably, by a suitable form of its $\mathcal{PT}$ symmetry, $\mathcal{C} = \mathcal{PTCPT}$.

3. Spectra

The structure of the above-mentioned general wavefunctions indicates that the singularities $x = 0$ and $z = (\pi/2) - x = 0$ remain the most suitable points where we can impose the boundary conditions. As long as they do not belong (by our assumption) to our complex curve of coordinates $\mathcal{C}(t)$, the choice and specification of these boundary conditions are not constrained by any (usually, obligatory) conditions of regularity.

One should still be careful in the classically forbidden domain of the very small couplings $\alpha > 0$ and $\beta > 0$. The related possible difficulties are well known. They represent a good reason for unnecessarily restrictive 'safe' postulates $A > 1$ and $B > 1$ as used by Flügge [4, p 89].

3.1. Refined boundary conditions

Once we discuss the specific ability of quantum mechanics which protects its systems from collapse into (sufficiently weak) attractive singularities, we have to eliminate superfluous solutions by all means including brute force [3, 5, 7]. In the present context, an application of the latter rule is significantly facilitated by our explicit knowledge (12) and (13) of the independent solutions in the leading-order approximation,

$$\psi(x) \sim x^{(1/2)\pm\beta} \quad x \ll 1 \qquad \psi(x) \sim \left(\tfrac{\pi}{2} - x\right)^{(1/2)\pm\alpha} \quad x \sim \tfrac{\pi}{2}. \tag{14}$$

Obviously, at the smallest couplings, these estimates remain compatible with the current boundary conditions $\psi(0) = \psi(\pi/2) = 0$ at an (almost) *arbitrary* positive energy E. A new paradox is derived. Even in the Hermitian case with $\varepsilon = 0$, the necessary physical reinstallation of the regularity must be achieved via the more restrictive boundary conditions

$$\lim_{x \to 0} \frac{\psi(x)}{\sqrt{x}} = 0 \qquad \beta \in \left(0, \tfrac{1}{2}\right) \tag{15}$$

(and, *mutatis mutandis*, for x near $\pi/2$; cf [9] for another solvable illustration of this rule).

In the present regularized $\mathcal{PT}$-symmetric generalization both the components in equation (14) remain equally acceptable. The situation is similar to the asymmetric but regular Hermitian models where one sometimes selects between the Dirichlet and Neumann (or, in general, mixed) boundary conditions. Here, at small couplings, any similar generalized requirements must be refined as well, working with limits similar to equation (15). Numerically, the situation will be badly ill-conditioned but we can still start from the fixed initial values of C_1 and C_2 at $x = 0$ and determine (a discrete set of) the energies E_n from another postulate of another fixed set of parameters $\tilde{C}^{(+)}$ and $\tilde{C}^{(-)}$ at $x = \pi/2$.

Similar 'weakly solvable' models, which do not require any termination of the hypergeometric series, also occur in applications from time to time [16]. We are not going to discuss them here in any detail.

3.2. Classification of exactly solvable cases

After our present regularization, one has to contemplate the whole infinite domain of $x(t)$ or $t \in (-\infty, \infty)$. Here we also omit this direction of considerations which generically leads to the Floquet theory and the characteristic band spectra for the $\mathcal{PT}$-symmetric and periodic systems [17].

In a narrower domain of applications related, for example, to attempts to generalize [18] or $\mathcal{PT}$ symmetrize [19] Calogero's three-body model [20], we solely pay attention to the problems which keep using the 'physical' boundary conditions imposed directly at the poles at $x = 0$ and $x = \pi/2$.

There exist several good practical reasons (e.g. the well-known slow convergence of the infinite hypergeometric series) for the exclusive preference of the terminating, polynomial Pöschl–Teller solutions. In such a setting, our explicit knowledge of the general solutions also facilitates complete classification of the eligible boundary conditions.

In the first step it is important to note that for the superposition (8), generically, the two necessary termination conditions are mutually incompatible. Fortunately, they differ just in one sign, $\sigma \to -\sigma$. Therefore, without any loss of generality we may put $C_2 = 0$ and write down the general termination condition

$$k = k_n^{(\sigma,\tau)} = \sigma\beta + \tau\alpha + 2n + 1 \qquad n = 0, 1, \ldots.$$

This reduces the infinite series (9) to the elementary Jacobi polynomial and, *simultaneously*, nullifies the cofactor G of the second subseries (11) in the alternative formula (10).

Summarizing, we are left with the unique elementary solution $\psi(x) = \psi_n^{(\sigma,\tau)}(x)$ with the energies $E_n^{(\sigma,\alpha)} = \left[k_n^{(\sigma,\tau)}\right]^2$ and wavefunctions

$$\psi_n^{(\sigma,\tau)}(x) = C_1 \sin^{(1/2)+\sigma\beta} x \cos^{(1/2)+\tau\alpha} x \,_2F_1(-n, n+1+\sigma\beta+\tau\alpha, 1+\sigma\beta; \sin^2 x).$$

Only our choice of the signs $\sigma = \pm 1$ and $\tau = \pm 1$ remains variable. In all these four cases there is no freedom left for our choice of the boundary conditions. By construction our solutions simply fit the $x \to 0$ rule

$$x^{-1/2}\psi^{(\sigma,\tau)}(x) = C_1 \, x^{\sigma\beta} + 0 \cdot x^{-\sigma\beta} \tag{16}$$

and its $x \to \pi/2$ parallel

$$z^{-1/2}\psi^{(\sigma,\tau)}(x) = C_1 \, G^{(\sigma,\tau)}(\pi/2 - x)^{\tau\alpha} + 0 \cdot (\pi/2 - x)^{-\tau\alpha}. \tag{17}$$

At every main quantum number $n = 0, 1, 2, \ldots$ we have a choice among the quadruplet of boundary conditions (16) and (17) giving the four different energy series

$$E_n^{(\sigma,\tau)} = \alpha^2 + \beta^2 + 2\sigma\tau\alpha\beta + (4n+2)(\sigma\beta + \tau\alpha) + (2n+1)^2$$

numbered by $\sigma = \pm 1$ and $\tau = \pm 1$. Two of them $\left(\text{cf } E_n^{(+,+)} = (\Sigma + 2n + 1)^2 \text{ and } E^{(-,-)} = (\Sigma - 2n - 1)^2\right)$ depend on the sum $\Sigma = \alpha + \beta$ and, in this sense, strongly resemble the Hermitian formula (2). The other two series $E_n^{(+,-)} = (\Delta + 2n + 1)^2$ and $E^{(-,+)} = (\Delta - 2n - 1)^2$ exhibit dependence on the mere difference $\Delta = \beta - \alpha$ and remain, unexpectedly, coupling-independent for the symmetric wells $V^{(B,B)}(x)$. In contrast, as already mentioned (cf figure 4), an interplay or superposition of the former two series provides one of the 'most natural' explanations of the paradox in figures 2 or 3.

Acknowledgment

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