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On the pseudo-norm and admissible solutions of the $\mathcal{PT}$-symmetric Scarf I potential

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Abstract
The physically admissible solutions of the $\mathcal{PT}$-symmetric Scarf I potential are identified in the domain of real and complex energies. It is found that generally there are no admissible complex-energy solutions, and there is one with real energy. In a limited range of the parameters there are two series of seemingly admissible solutions both with the real and complex energies belonging to quasi-parity $q = \pm$; however, the two sets are not $\mathcal{PT}$-orthogonal in the domain of real energies. The sign of the pseudo-norm of states with real energy is found to oscillate as $(-1)^n$, in accordance with the example of other $\mathcal{PT}$-symmetric potentials possessing an infinite number of discrete levels. It is argued that the spontaneous breakdown of $\mathcal{PT}$-symmetry cannot be defined for the Scarf I potential. A comparison with some $\mathcal{PT}$-symmetric extensions of the infinite square well is presented.

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1. Introduction

The introduction of $\mathcal{PT}$-symmetric quantum mechanics [1] generated renewed interest in the analysis of quantum mechanical potentials including their physically relevant solutions, their energy spectrum and generally their physical and mathematical interpretation. $\mathcal{PT}$-symmetric Hamiltonians are required to be invariant under the simultaneous action of space ($\mathcal{P}$) and time ($\mathcal{T}$) reversal. Most efforts have been devoted to the study of the Schrödinger equation in one dimension, in which case $\mathcal{PT}$-symmetry means allowing complex potentials obeying the $V^*(-x) = V(x)$ relation, i.e. their real and imaginary components are even and odd functions of the coordinate x, respectively. These manifestly non-Hermitian systems mimic several features of Hermitian ones. Perhaps the most notable of these is that their energy spectrum may consist partly or fully of real energy eigenvalues. Further features not expected from complex potentials were the conservation of the norm and the orthogonality of the states;

however, for this the conventional inner product $\langle\psi_n|\psi_l\rangle$ had to be replaced with the $\mathcal{PT}$-inner product $\langle\psi_n|\mathcal{P}|\psi_l\rangle$.

Another remarkable phenomenon was that tuning some parameter (generally such that non-Hermiticity increased) resulted in the pairwise merging of real energy eigenvalues and their re-emergence as complex conjugate pairs. This phenomenon was interpreted as the spontaneous breakdown of $\mathcal{PT}$-symmetry [1], and it was also found that not all $\mathcal{PT}$-symmetric potentials can undergo this process.

A major development was the identification of $\mathcal{PT}$-symmetry as a special case of pseudo-Hermiticity [2], which explained many unusual features of $\mathcal{PT}$-symmetric quantum mechanics. A Hamiltonian H is said to be η-pseudo-Hermitian, if there exists a linear, Hermitian, invertible operator η for which it satisfies the relation $H^\dagger = \eta H\eta^{-1}$. This also implies the redefinition of the inner product as $\langle\psi_n|\eta|\psi_l\rangle$. This construction contains both conventional Hermiticity ($\eta = 1$) and $\mathcal{PT}$-symmetry ($\eta = \mathcal{P}$) as a special case.

A further natural requirement was investigating the relation between $\mathcal{PT}$-symmetric (or, in general, pseudo-Hermitian) Hamiltonians and their possible Hermitian equivalents [3, 4]. In practical terms this required the modification of the inner product such that the norm is restored to positive values, allowing for the probabilistic interpretation of the wavefunctions. This required the introduction of the $\mathcal{C}$ charge operator [5]. It is notable that the question of the physically consistent description of non-Hermitian Hamiltonians in terms of a modified metric has been discussed well before [6] the introduction of $\mathcal{PT}$-symmetric quantum mechanics.

Although it appears in numerous derivations in an abstract form, the pseudo-norm is known only for a few concrete cases. It is generally assumed to show oscillatory behaviour $(-1)^n$ with respect to the principal quantum number n, as e.g. for a $\mathcal{PT}$-symmetric square well [4]. More recently, this pattern was proven exactly [7] for a class of potentials that are written in a polynomial form of $\mathrm{i}x$ (including some anharmonic oscillators and the archetype of $\mathcal{PT}$-symmetric potentials, $V(x) = \mathrm{i}x^3$, for example). However, there is at least one counter-example, since the pseudo-norm of the $\mathcal{PT}$-symmetric Scarf II potential is known to deviate from the oscillatory trend [8]. This potential is rather different from those mentioned above both in its shape (finite depth and infinite range) and energy spectrum (finite number of discrete levels). It is thus reasonable to investigate the pseudo-norm in the $\mathcal{PT}$-symmetric Scarf I potential, the trigonometric analogue of the Scarf II potentials: first its mathematical structure is close to that of the Scarf II potential, and second, its physical nature resembles the potentials for which the pseudo-norm alternates with n.

In section 2 we discuss the $\mathcal{PT}$-symmetric Scarf I potential in various parameter ranges corresponding to different types of singularities and identify the admissible solutions for real and complex energies. We calculate the pseudo-norm for these states and discuss the transition between the domains with real and complex energies. In section 3 we summarize the results and give a brief comparison of the $\mathcal{PT}$-symmetric Scarf I potential with some $\mathcal{PT}$-symmetric extensions of the square-well potential.

2. The $\mathcal{PT}$-symmetric Scarf I potential

The general form of the Scarf I potential is [9, 10]

$$V(x) = \left(\frac{\alpha^2+\beta^2}{2} - \frac{1}{4}\right)\frac{1}{\cos^2(x)} + \frac{\alpha^2-\beta^2}{2}\frac{\sin(x)}{\cos^2(x)}, \tag{1}$$

where $x \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$. Introducing a new variable

$$z = \frac{1-\sin x}{2} \tag{2}$$

the general solutions are given in terms of hypergeometric functions [11] as

$$\psi^{(+)}(x) \sim [z(x)]^{\frac{\alpha}{2}+\frac{1}{4}}[1-z(x)]^{\frac{\beta}{2}+\frac{1}{4}} F\left(\frac{\alpha+\beta+1}{2}-k, \frac{\alpha+\beta+1}{2}+k; \alpha+1; z(x)\right) \tag{3}$$

and

$$\psi^{(-)}(x) \sim [z(x)]^{-\frac{\alpha}{2}+\frac{1}{4}}[1-z(x)]^{-\frac{\beta}{2}+\frac{1}{4}} F\left(\frac{-\alpha-\beta+1}{2}-k, \frac{-\alpha-\beta+1}{2}+k; -\alpha+1; z(x)\right), \tag{4}$$

where $E = k^2$. Note that (3) and (4) are interrelated via $\alpha, \beta \leftrightarrow -\alpha, -\beta$. We make use of this finding in identifying the two solutions by the indices '+' and '−'. There are also further ways of writing the two independent solutions due to the rich variety of transformation formulae concerning the hypergeometric function [11].

When the first or second argument of the hypergeometric functions in (3) or (4) is a non-positive integer $-n$, then these functions turn into Jacobi polynomials and formally discrete energy eigenvalues can be obtained:

$$E_n^{(\pm)} = \left(n + \frac{\pm\alpha + \pm\beta + 1}{2}\right)^2. \tag{5}$$

However, these solutions are not necessarily physical, as this depends on the boundary conditions too. A physically acceptable solution should vanish at the boundaries, and considering the finite domain of definition, this also implies its square integrability. Since according to (2) $x = \pm\frac{\pi}{2}$ correspond to $z = 1$ and $z = 0$, where the hypergeometric function takes on the finite value [11], the regularity or singularity of the solutions depends on the trigonometric prefactors in (3) and (4), and in particular, on α and β. It can be shown that the behaviour of the two solutions near the boundaries is

$$\lim_{x\to-\pi/2} \psi^{(\pm)}(x) \sim r^{\pm\beta+\frac{1}{2}} \tag{6}$$

and

$$\lim_{x\to\pi/2} \psi^{(\pm)}(x) \sim r^{\pm\alpha+\frac{1}{2}}, \tag{7}$$

where $r = \frac{\pi}{2} \pm x$. The potential itself behaves there as $V\left(x \to -\frac{\pi}{2}\right) \sim \left(\beta^2 - \frac{1}{4}\right)r^{-2}$, and $V\left(x \to \frac{\pi}{2}\right) \sim \left(\alpha^2 - \frac{1}{4}\right)r^{-2}$, so it exhibits various types of singularity, depending on α and β.

Before specifying the general formulae for the $\mathcal{PT}$ Scarf I potential, we note that the conventional (Hermitian) Scarf I potential is obtained if α and β are real. In this case $\psi^{(+)}(x)$ is regular if $\alpha, \beta > -\frac{1}{2}$ holds, while the same condition for $\psi^{(-)}(x)$ is $\alpha, \beta < \frac{1}{2}$. For $\alpha, \beta = \pm\frac{1}{2}$ (which corresponds to the infinite square well) both solutions are regular, but one of them takes on the finite value at the boundaries. This means that, in general, only one of the solutions can be physical; however, in the domain $-\frac{1}{2} < \alpha, \beta < \frac{1}{2}$ both solutions are square integrable and fulfil the boundary conditions $\psi\left(\pm\frac{\pi}{2}\right) = 0$. This corresponds to weakly attractive inverse square-type singularities [12], which means that $V(r) \sim \gamma r^{-2}$ with $-\frac{1}{4} < \gamma < 0$. In this case the usual procedure is keeping the less singular solution as the physical one and discarding the other one. This intuitive choice is also supported by a mathematically more well-founded argument based on the theory of the self-adjoint extension of operators [12].

In order to make (1) $\mathcal{PT}$-symmetric α and β have to be chosen complex such that $\beta^* = \pm\alpha$ [9, 10]. Besides this, the discussion presented up to this point remains valid; however, there are some further aspects that are specific to $\mathcal{PT}$-symmetry, such as the different definition of the inner product. One further aspect is that an imaginary coordinate shift can also be applied, and in contrast with a possible real coordinate shift for the real problem, it changes the potential in an essential way [9, 10], e.g. by cancelling its singularities. However, we do not consider this option here.

2.1. Solutions with real energy: $\beta = \alpha^*$

The energy eigenvalues (5) take on real values for $\beta = \alpha^*$, i.e. for $\beta_R = \alpha_R$ and $\beta_I = -\alpha_I$, where $\alpha = \alpha_R + \mathrm{i}\alpha_I$ and $\beta = \beta_R + \mathrm{i}\beta_I$. The singularity of the potential at the boundaries is formally the same as in the general case; however, now the coefficients setting the strength of the singularities are complex: $\alpha_R^2 - \alpha_I^2 - \frac{1}{4} \mp \mathrm{i}2\alpha_R\alpha_I$ at $x = \pm\frac{\pi}{2}$. Equations (6) and (7) are also valid; however, it is now α_R that determines whether the solutions are regular or singular at the boundaries. In what follows we shall discuss the cases $|\alpha_R| > \frac{1}{2}$, $|\alpha_R| = \frac{1}{2}$ and $|\alpha_R| < \frac{1}{2}$ separately, because the two solutions have different pattern of singularities in these domains. In fact, without loss of generality it is enough to study α_R on the half axis (say, for $\alpha_R \geqslant 0$), because the two solutions simply exchange roles if the $\alpha \leftrightarrow -\alpha$ (and thus the $\beta \leftrightarrow -\beta$) choice is made.

Let us assume that $\alpha_R > \frac{1}{2}$ holds, which implies that (3) is regular and (4) is singular. The physical wavefunctions can then be written in terms of Jacobi polynomials:

$$\psi_n^{(+)}(x) = D_n^{(+)}(1-\sin x)^{\frac{\alpha}{2}+\frac{1}{4}}(1+\sin x)^{\frac{\alpha^*}{2}+\frac{1}{4}} P_n^{(\alpha,\alpha^*)}(\sin x). \tag{8}$$

Based on the properties of the Jacobi polynomials [11] it is easy to show that (8) is an eigenfunction of the $\mathcal{PT}$ operator with eigenvalue $(-1)^n\big(D_n^{(+)}\big)^*\big/D_n^{(+)}$, i.e. with eigenvalue 1 if the normalization constant is chosen as

$$D_n^{(+)} = \mathrm{i}^n d_n^{(+)}, \qquad d_n^{(+)} \in R. \tag{9}$$

In determining the normalization constant and the pseudo-norm we follow the procedure presented in [8] for the Scarf II potential. For this we calculate the general $\mathcal{PT}$-inner product of two wavefunctions:

$$I_{nl}^{(++)} \equiv \big\langle\psi_n^{(+)}\big|\mathcal{P}\big|\psi_l^{(+)}\big\rangle = \int_{-\pi/2}^{\pi/2}\psi_n^{(+)}(x)\big[\psi_l^{(+)}(-x)\big]^*\,\mathrm{d}x. \tag{10}$$

The first step is rewriting the Jacobi polynomials in terms of explicit sums as [11]

$$P_n^{(\alpha,\beta)}(\sin x) = \frac{1}{2^n}\sum_{m=0}^{n}\binom{n+\alpha}{m}\binom{n+\beta}{n-m}(-1)^{n-m}(1-\sin x)^{n-m}(1+\sin x)^m \tag{11}$$

remembering that $\beta = \alpha^*$ holds. Then we apply the integral formula [13]

$$\int_{-\pi/2}^{\pi/2}(1-\sin x)^p(1+\sin x)^q\,\mathrm{d}x = 2^{p+q}\frac{\Gamma\big(p+\frac{1}{2}\big)\Gamma\big(q+\frac{1}{2}\big)}{\Gamma(p+q+1)} \tag{12}$$

term by term in equation (10). This can be done if $\mathrm{Re}(p), \mathrm{Re}(q) > -\frac{1}{2}$ holds, which is always the case here. Then a double sum formula is obtained:

$$\begin{aligned} I_{nl}^{(++)} = {} & D_n^{(+)}\big[D_l^{(+)}\big]^*(-1)^{n+l}2^{\alpha+\alpha^*+1} \\ & \times\sum_{m=0}^{n}(-1)^m\binom{n+\alpha}{m}\binom{n+\alpha^*}{n-m}\sum_{i=0}^{l}(-1)^i\binom{l+\alpha^*}{i}\binom{l+\alpha}{l-i} \\ & \times\frac{\Gamma(\alpha+n-m+i+1)\Gamma(\alpha^*+l-i+m+1)}{\Gamma(\alpha+\alpha^*+n+l+2)} \end{aligned} \tag{13}$$

$$= D_n^{(+)}\left[D_l^{(+)}\right]^* \frac{\sin[(\alpha+\alpha^*)\pi]}{2\sin(\alpha\pi)\sin(\alpha^*\pi)} Q_{nl}^{(\alpha,\alpha^*,\alpha,\alpha^*)} \tag{14}$$

$$= \delta_{nl}(-1)^n \left|D_n^{(+)}\right|^2 \frac{2^{\alpha+\alpha^*+1}}{\alpha+\alpha^*+2n+1} \frac{\Gamma(\alpha+n+1)\Gamma(\alpha^*+n+1)}{n!\Gamma(\alpha+\alpha^*+n+1)}. \tag{15}$$

Here (14) follows from a formula appearing in the analogous process applied to the Scarf II potential [8]. It is remarkable that although in the actual integrations there hyperbolic functions appear, rather than trigonometric ones, still the summation reduces to a similar formula evaluated explicitly in (15).

Equation (15) clearly demonstrates the expected $\mathcal{PT}$-orthogonality of the wavefunctions with $n \neq l$, and it also gives a closed explicit formula for the pseudo-norm for $n = l$. The analysis of the individual terms of (15) shows that the pseudo-norm is real: the reality of most terms is trivial, while the two gamma functions in the numerator are each other's complex conjugate, so their product is also real. Furthermore, it is also seen that due to the assumption $\alpha_R > \frac{1}{2}$ the sign of the pseudo-norm $I_{nn}^{(++)}$ is determined by the $(-1)^n$ term, i.e. it oscillates with n. This behaviour of the pseudo-norm is similar to that observed for other $\mathcal{PT}$-symmetric potentials possessing infinite number of discrete levels and differs from, e.g., the example of the Scarf II potential [8], which has finite number of discrete levels. In addition to the $(-1)^n$ factor, in the latter case the sign of the pseudo-norm is also influenced by gamma functions depending on $-n$ among other parameters, and this leads to deviations from the oscillatory trend.

The actual expression of the normalization constant, considering also (9), is

$$D_n^{(+)} = \mathrm{i}^n \left(\frac{(2n+2\alpha_R+1)n!\Gamma(n+2\alpha_R+1)}{2^{2\alpha_R+1}\Gamma(n+\alpha+1)\Gamma(n+\alpha^*+1)} \right)^{1/2}. \tag{16}$$

It is notable that apart from the i^n factor this expression can be obtained from the normalization constant of the real Scarf I case by formally substituting *complex* values into the *real* α and β parameters. It has to be stressed that the Jacobi polynomials, and in particular, the standard integration formula they satisfy are defined normally for real values of α and β [11].

Let us now turn to the intermediate zone $-\frac{1}{2} < \alpha_R < \frac{1}{2}$, where both (3) and (4) vanish at $x = \pm\frac{\pi}{2}$, and thus are normalizable. In fact, equations (15) and (16) are valid for $\psi_n^{(+)}(x)$ in this range too, because the integration formula (12) is applicable up to $\alpha_R > -1$ (which includes even some irregular, though normalizable solutions in the range $-\frac{1}{2} > \alpha_R > -1$). Actually, it can be shown that the oscillatory behaviour of $I_{nn}^{(++)}$ persists for $\alpha_R > -\frac{1}{2}$ too. This can be proven trivially for $n > 0$, because all the individual real terms mentioned above are positive then, while for $n = 0$ the two terms in the denominator can be combined to yield a positive expression as $(2\alpha_R+1)\Gamma(2\alpha_R+1) = \Gamma(2\alpha_R+2) > 0$, since $2\alpha_R+2 > 1$ holds. The equivalent formulae $I_{nn}^{(--)}$ and $D_n^{(-)}$ for the second solution $\psi_n^{(-)}(x)$ can be obtained trivially by replacing α with $-\alpha$ (and thus α_R with $-\alpha_R$).

These results indicate that similar to some other solvable $\mathcal{PT}$-symmetric potentials a quasi-parity quantum number $q = \pm$ could also be defined through $q\alpha$ (and thus $q\beta$) too, at least in the limited parameter range $|\alpha_R| < \frac{1}{2}$. Due to this choice q would appear only in the energy eigenvalues and the wavefunctions, but obviously, would not influence the potential function (1) itself. In what follows we investigate this possibility.

Given the two normalizable solutions in this limited range of α_R the question whether they form orthogonal sets arises naturally. Generally there is an indirect proof for this in the case of $\mathcal{PT}$-symmetric potentials using the formula

$$\left(E_n^{(q)} - \left[E_l^{(p)}\right]^*\right) \int_a^b \psi_n^{(q)}(x)\left[\psi_l^{(p)}(-x)\right]^* \mathrm{d}x = 0, \tag{17}$$

which is obtained from the Schrödinger equations satisfied by the two wavefunctions and making use of the $\mathcal{PT}$-symmetry of $V(x)$. Equation (17) indicates that the integral has to vanish whenever the two energy eigenvalues are different, which is clearly the case if the quasi-parities q and p are different. However, equation (17) is applicable only if the wavefunctions *and their derivatives* vanish at the boundaries $x = a$ and b. This assumption is not valid in the case of the Scarf I potential, where the equivalent of (17) is

$$\left(E_n^{(+)} - \left[E_l^{(-)}\right]^*\right) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \psi_n^{(+)}(x)\left[\psi_l^{(-)}(-x)\right]^* \mathrm{d}x = \left[\psi_n^{(+)}(x)\frac{\mathrm{d}\left[\psi_l^{(-)}(-x)\right]^*}{\mathrm{d}x} - \left[\psi_l^{(-)}(-x)\right]^* \frac{\mathrm{d}\psi_n^{(+)}(x)}{\mathrm{d}x}\right]_{-\pi/2}^{\pi/2}. \tag{18}$$

Note that even if the wavefunctions vanish at the boundaries, their derivatives need not, so the expression on the right-hand side need not be zero as in the case of other $\mathcal{PT}$-symmetric potentials. Substituting the expressions for the wavefunctions and the energy eigenvalues and taking the limits $x \to \pm\frac{\pi}{2}$ (including also the application of the l'Hospital rule) we obtain the expression

$$I_{nl}^{(+-)} = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \psi_n^{(+)}(x)\left[\psi_l^{(-)}(-x)\right]^* \mathrm{d}x = \frac{2D_n^{(+)}\left[D_l^{(-)}\right]^*}{(n+l+1)(n-l+2\alpha_R)} \times \left[(-1)^l\alpha\binom{n+\alpha}{n}\binom{l-\alpha}{l} + (-1)^n\alpha^*\binom{n+\alpha^*}{n}\binom{l-\alpha^*}{l}\right]. \tag{19}$$

This expression is not zero in general, so we conclude that the two sets of regular solutions occurring in the limited parameter range $|\alpha_R| < \frac{1}{2}$ do not form $\mathcal{PT}$-orthogonal sets. We note that an alternative equation can also be derived for the integral (19) by substituting directly the expression for the wavefunctions $\psi_n^{(+)}(x)$ and $\psi_l^{(-)}(x)$ in (8). Then a formula resembling (13) is obtained:

$$I_{nl}^{(+-)} = 2D_n^{(+)}\left[D_l^{(-)}\right]^*(-1)^{n+l} \times \sum_{m=0}^{n}(-1)^m\binom{n+\alpha}{m}\binom{n+\alpha^*}{n-m}\sum_{i=0}^{l}(-1)^i\binom{l-\alpha^*}{i}\binom{l-\alpha}{l-i} \times \frac{(n-m+i)!(l-i+m)!}{(n+l+1)!}. \tag{20}$$

Although the exact proof of the equivalence of (20) and (19) is not obvious, they lead to the same results for the first few values of n and l. Note that $I_{nl}^{(+-)} \neq I_{ln}^{(+-)}$.

It is notable that a similar situation occurs in real potentials with weakly attractive γr^{-2}-type singularity (i.e. for $-\frac{1}{4} < \gamma < 0$): then both solutions are normalizable; furthermore, they even vanish at the singularity [12]. As has been mentioned earlier, in this case the less singular solution is kept as the physical one, which is also the option supported by the theory of the self-adjoint extension of operators [12]. Although the concept of a physically admissible state is less well defined in the case of $\mathcal{PT}$-symmetric potentials, similar to the Hermitian problems, it would be reasonable to consider only one of the normalizable solutions as the physical one. The question whether this choice could be justified by more well-founded arguments, such as generalizing the concept of self-adjoint extension of Hamiltonians to $\mathcal{PT}$-symmetric (complex) potentials is beyond the scope of the present work.

Finally, let us investigate the transitional situation with $\alpha_R = \pm\frac{1}{2}$. This situation is similar to the case of $|\alpha_R| > \frac{1}{2}$ in that only one of the solutions can be accepted as physical: although the other one is not infinite at the boundaries, rather it takes on the finite value there and thus still cannot be accepted. The situation is similar to the real infinite square well (corresponding to $\alpha = \beta = \pm\frac{1}{2}$): the solutions with $\alpha = \beta = \frac{1}{2}$ vanish at the boundaries and thus are physical, while those with $\alpha = \beta = -\frac{1}{2}$ are normalizable and finite at the boundaries (e.g. the constant function at $n = 0$), but cannot be considered physical.

2.2. Solutions with complex energy: $\beta = -\alpha^*$

If the $\beta = -\alpha^*$ choice is made, the energy eigenvalues (5) become complex; furthermore, the energies belonging to the two solutions (3) and (4) form complex conjugate pairs. It is thus tempting to interpret this situation as the Scarf I potential with spontaneously broken $\mathcal{PT}$-symmetry. Before inspecting this possibility, let us first discuss whether the boundary conditions allow physically admissible solutions in this case.

It turns out that for $|\alpha_R| > \frac{1}{2}$ both solutions vanish at one boundary, but become singular at the other, so they cannot be considered physically acceptable. For $|\alpha_R| = \frac{1}{2}$ the singularity vanishes; however, the solution still takes on the finite value at the boundary, so it remains physically unacceptable. It is known that the two solutions cease to be $\mathcal{PT}$-symmetric in these cases; rather they are connected by the $\mathcal{PT}$ operator, and this explains why they have different behaviour at the two boundaries, in contrast with the solutions in the case with unbroken $\mathcal{PT}$-symmetry.

The only situation when both solutions vanish at both boundaries occurs for $-\frac{1}{2} < \alpha_R < \frac{1}{2}$, which is also the domain where there were two vanishing solutions in the case of unbroken $\mathcal{PT}$-symmetry. In this case the two solutions can be written in terms of Jacobi polynomials. It is notable that the energies associated with these two solutions, $E_n^{(\pm)} = \left(n + \frac{1}{2} \pm \mathrm{i}\alpha_I\right)^2$, do not depend on the crucial α_R parameter.

Let us now investigate the transition between the domains of real and complex energy eigenvalues, i.e. the situations with $\beta = \alpha^*$ and $\beta = -\alpha^*$. The transition clearly has to go through the critical point $\alpha = \beta = 0$, which corresponds to the real, symmetric and singular potential $V(x) = -\frac{1}{4}\cos^{-2}x$. This potential has transitional-type attractive singularity at both boundaries with $V(x) \sim -\frac{1}{4}r^{-2}$ $\left(r = \frac{\pi}{2} \pm x\right)$, which is considered as the entrance to the case of the particle falling into the centre of attraction [12]. This scenario is in obvious contrast with the smooth transition observed in other $\mathcal{PT}$-symmetric potentials.

It is also remarkable that continuing the two solutions (with $q = \pm$) to the domain of unbroken symmetry we face with the problem discussed in subsection 2.1, i.e. that they do not form a $\mathcal{PT}$-orthogonal set. All these arguments together indicate that the spontaneous breakdown of $\mathcal{PT}$-symmetry cannot be defined in the Scarf I potential.

3. Summary and outlook

With the intention of determining the pseudo-norm of its states, we investigated the $\mathcal{PT}$-symmetric version of the Scarf I potential (1) and identified its physically admissible solutions. This potential has $\left(\frac{\pi}{2} \mp x\right)^{-2}$-type singularity at the boundaries $x = \pm\frac{\pi}{2}$ (unless an imaginary coordinate shift $x \to x + \mathrm{i}\varepsilon$ is applied), and it turned out that these singularities restrict the admissible solutions considerably.

The Scarf I potential is $\mathcal{PT}$-symmetric if either $\beta = \alpha^*$ or $\beta = -\alpha^*$ holds. In both cases it is $\alpha_R = \mathrm{Re}(\alpha)$ that determines whether the solutions vanish at the boundaries, or they take on a finite or infinite value there. For $|\alpha_R| \geqslant \frac{1}{2}$ there are no physically admissible solutions for $\beta = -\alpha^*$, while for $\beta = \alpha^*$ one of them is admissible (i.e. vanishes at both boundaries) and it corresponds to real energy eigenvalues. This indicated that the spontaneous breakdown of the $\mathcal{PT}$-symmetry of the Scarf I potential cannot occur in this parameter range. For $-\frac{1}{2} < \alpha_R < \frac{1}{2}$, in principle, there are two admissible solutions in both cases with real and complex energies for $\beta = \alpha^*$ and $\beta = -\alpha^*$, respectively. However, the problems here arise in the domain of real energies ($\beta^* = \alpha$), as it turned out that the two sets of wavefunctions $\psi_n^{(+)}(x)$ and $\psi_n^{(-)}(x)$ do not form an orthogonal set with respect to the $\mathcal{PT}$-inner product. Based on the analogy with real potentials possessing attractive r^{-2}-type singularity, it seems reasonable to keep only one of the solutions as physical in this case. These findings together with the fact that the transition between the domain of real and complex energies must occur through $\alpha = \beta = 0$, which corresponds to the singular $V(x) = -\frac{1}{4}\sec^2 x$ potential, we concluded that the spontaneous breakdown of $\mathcal{PT}$-symmetry cannot be defined for the Scarf I potential.

We calculated the pseudo-norm of the admissible solutions for the $\beta = \alpha^*$ case and found that it oscillates with the principal quantum number as $(-1)^n$. This is similar to the situation with other $\mathcal{PT}$-symmetric potentials with infinite number of discrete levels, but differs from the example of the $\mathcal{PT}$-symmetric Scarf II potential, the hyperbolic analogue of the (trigonometric) Scarf I potential.

An interesting special case of the $\mathcal{PT}$-symmetric Scarf I potential occurs for $\alpha_I^2 = \alpha_R^2 - \frac{1}{4}$, which leads to a one-parameter $\mathcal{PT}$-symmetric extension of the infinite square well:

$$V(x) = \pm 2\mathrm{i}\,\alpha_R \left(\alpha_R^2 - \frac{1}{4}\right)^{1/2} \frac{\sin(x)}{\cos^2(x)}. \tag{21}$$

Obviously, only those solutions can be admitted that vanish at the boundaries $x = \pm\frac{\pi}{2}$. Since $|\alpha_R| \geqslant \frac{1}{2}$ has to be satisfied, similar to the general case, only one of the solutions will be physically acceptable, and only in the case corresponding to real energy eigenvalues, i.e. $\beta = \alpha^*$. These results imply that similar to the general $\mathcal{PT}$-symmetric Scarf I potential the spontaneous breakdown cannot occur for the potential (21). This is in contrast with other types of the $\mathcal{PT}$-symmetric square-well potential. These include examples where the imaginary component is an odd step function with one [4, 10, 14] or two steps [15], or a combination of δ functions [16]. This difference might occur due to the singularity of the imaginary potential in (21).

Finally, the analogy with real singular potentials raises the question whether there is a way to generalize the concept of the self-adjoint extension of Hamiltonians to $\mathcal{PT}$-symmetric, and in general, pseudo-Hermitian systems. Similar to real potentials, this problem is exposed by the handling of solutions with proper boundary conditions, and in particular, selecting the 'physical' one when there are several solutions that are square integrable and vanish at the boundaries. In the real case the self-adjoint extension is implemented through a regularization procedure [12] that selects the less singular solution. The adaptation of this method to $\mathcal{PT}$-symmetric (pseudo-Hermitian) systems would certainly be worthwhile.

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