PT symmetry breaking and explicit expressions for the pseudo-norm in the Scarf II potential

G. Lévai
\( ^a \) Institute of Nuclear Research of the Hungarian Academy of Sciences, PO Box 51, H–4001 Debrecen, Hungary

F. Cannata
\( ^b \) Dipartimento di Fisica dell'Università and Istituto Nazionale di Fisica Nucleare, I-40126 Bologna, Italy

A. Ventura
\( ^c \) Ente Nuove Tecnologie, Energia e Ambiente, Bologna, Italy

Abstract

Closed expressions are derived for the pseudo-norm, norm and orthogonality relations for arbitrary bound states of the \( PT \) symmetric and the Hermitian Scarf II potential for the first time. The pseudo-norm is found to have indefinite sign in general. Some aspects of the spontaneous breakdown of \( PT \) symmetry are analysed.

Key words: Solvable potentials, spontaneous breakdown of \( PT \) symmetry, pseudo-norm, orthogonality

PACS: 03.65.Ge, 02.30.-f, 11.30.Qc

1 Introduction

Non-Hermitian quantum mechanical problems have attracted much attention recently. The main reason for this is that the energy spectrum of a number of complex potentials turned out to be real (at least partly), which contradicted the usual expectations regarding non-Hermitian systems. Strangely enough,
the first examples for complex potentials with real spectra were found using numerical techniques [1]. This unusual behaviour of the energy spectrum was attributed to the so-called $PT$ symmetry, i.e. the invariance of the Hamiltonian with respect to the simultaneous space ($P$) and time ($T$) reflection. For one-dimensional potential problems this requires $[V(-x)]^* = V(x)$, which implies that the real component of the potential must be an even function of $x$, while the imaginary component has to be odd. After the first examples, further ones have been identified using semiclassical [2], numerical [3] and perturbative [4] methods, and a number of exactly solvable $PT$ symmetric potentials have also been found, mainly as the analogues of Hermitian (real) potentials [5–7].

It was also noticed that $PT$ symmetry is neither a necessary, nor a sufficient condition for having real energy spectrum in a complex potential. It is not a necessary condition, because there are complex non-$PT$ symmetric potentials with these properties: some of these are complex supersymmetric partners of real potentials [8], while some others can be obtained by merely shifting $PT$ symmetric potentials along the $x$ axis, which (formally) cancels $PT$ symmetry, but obviously does not influence the energy spectrum. Neither is $PT$ symmetry a sufficient condition, because complex-energy solutions of such potentials are also known, and since in this case the energy eigenfunctions cease to be eigenfunctions of the $PT$ operator, this scenario has been interpreted as the spontaneous breakdown of $PT$ symmetry [1]. No general condition has been found for the breakdown of $PT$ symmetry, but it has been observed that it usually characterizes strongly non-Hermitian problems [1,9–11].

Obviously, the lack of Hermiticity raises questions about the probabilistic interpretation of the wavefunctions (probability density, continuity equation), and in general, about the definition of the norm and the inner product of the eigenvectors of the non-Hermitian Hamiltonian. It has been suggested, for example, that the $\psi^2(x)$ quantity should replace $|\psi(x)|^2$ in the definition of the norm [12]. For unbroken $PT$ symmetry this expression coincides with the $\psi(x)\psi^*(-x)$ quantity used in the definition of the pseudo-norm [13], which is obtained from the modified inner product $\langle \psi_1 | P | \psi_2 \rangle$. This redefinition of the inner product was found to lead to the orthogonality of the energy eigenstates, but it also resulted in an indefinite metric, replacing the usual Hilbert space with the Krein space [14]. Efforts have been made to restore the Hermitian formalism using projection techniques [13,14].

Exactly solvable examples can be extremely useful in the understanding of the unusual features of $PT$ symmetric problems and the underlying new physical concepts. For example, by the continuous tuning of the potential parameters through critical values the mechanism of $PT$ symmetry breaking can be studied; conditions for positive and negative values of the pseudo-norm can be identified, etc. Although a number of exactly solvable $PT$ symmetric po-
tentials have been identified, these questions have been addressed only in very few cases.

The Scarf II (sometimes also called hyperbolic Scarf or Gendenshtein) potential is in a special position among exactly solvable potentials. This shape-invariant potential [15] is defined on the whole $x$ axis, it has no singularity at $x = 0$, and in contrast with most other shape-invariant potentials, it can be turned into a $PT$ symmetric form without regularizing its singularity by means of an $x \to x + i\epsilon$ imaginary coordinate shift [6,16]. Therefore it is not surprising that it became a “guinea pig” of testing $PT$ symmetry on a solvable example. It has been associated with the $sl(2,C)$ [17], $su(1,1)\approx so(2,1)$ [18] and $so(2,2)$ [19] potential algebras, and it has also been observed that its $PT$ symmetric version has a second set of bound states, which appear as resonances in its Hermitian version [17,18]. This mechanism of doubling the bound states is essentially different from the one arising from the cancellation of singularities at $x = 0$ by the imaginary coordinate shift. This potential is also known to have (purely) real and (purely) complex energy spectrum, depending on the relative strength of its real and imaginary component [9], and since the two domains can be connected with a continuous tuning of the parameters without crossing a singularity, it is a perfect example to illustrate the breakdown of $PT$ symmetry.

It would also be a suitable example to illustrate the modified definition of the inner product and the behaviour (sign) of the pseudo-norm, and the other implications for the use of the Krein space instead of the usual Hilbert space, however, there is a major obstacle: the evaluation of integrals involving them could not be calculated as yet analytically, except for the ground state [20]. In fact, even an explicit proof of the orthogonality of the bound states is missing, both for the Hermitian [21], and the $PT$ symmetric case [9]. In the latter case only indirect proof has been given for orthogonality of some states [9].

Obviously, the evaluation of integrals containing the energy eigenfunctions of the Scarf II potential is essential to complete the analysis of this perfect example for $PT$ symmetry, i.e. to study the behaviour of the pseudonorm and to prove the orthogonality of the eigenstates in general. In this Letter we present a method to evaluate these integrals for the first time, both for the $PT$ symmetric and the Hermitian version of the Scarf II potential, and use these results to illustrate the mechanism of $PT$ symmetry breaking. In particular, we prove the orthogonality of the eigenstates and derive the normalization constants (the norm) both for the $PT$ symmetric and the Hermitian version of this potential, and also analyse the $PT$ symmetric case as a conventional complex potential, using the standard (Hilbert space) definition of the inner product.
2 The general form of the Scarf II potential

Here we follow the notation of Refs. [6,22] to discuss the Scarf II potential

\[ V(x) = -\frac{1}{\cosh^2(x)} \left[ \left( \frac{\alpha + \beta}{2} \right)^2 + \left( \frac{\alpha - \beta}{2} \right)^2 - \frac{1}{4} \right] \]

\[ + 2i \frac{\sinh(x)}{\cosh^2(x)} \left( \frac{\beta + \alpha}{2} \right) \left( \frac{\beta - \alpha}{2} \right). \]

The bound-state energy eigenvalues are

\[ E_{n}^{(\alpha,\beta)} = -\left( n + \frac{\alpha + \beta + 1}{2} \right)^2, \]

while the corresponding wavefunctions

\[ \psi_{n}^{(\alpha,\beta)}(x) = C_{n}^{(\alpha,\beta)} (1 - i \sinh(x))^{\frac{\alpha}{2} + \frac{1}{4}} (1 + i \sinh(x))^{\frac{\beta}{2} + \frac{1}{4}} P_{n}^{(\alpha,\beta)}(i \sinh(x)) \]

are expressed in terms of Jacobi polynomials [23] and are normalizable if \( n < -[\text{Re}(\alpha + \beta) + 1]/2 \) holds.

In the Hermitian case \( \alpha \) and \( \beta \) are complex and satisfy \( \alpha^* = \beta, \beta = -s - \frac{1}{2} - i\lambda, \beta = -s - \frac{1}{2} + i\lambda [21,24] \). In this case only one regular solution exists. With arbitrary \( \alpha \) and \( \beta \) obviously, the general complex version of the Scarf II potential is obtained.

The Scarf II potential can be made \( PT \)-symmetric if \( \alpha^* = \pm \alpha \) and \( \beta^* = \pm \beta \) holds [6], i.e. if \( \alpha \) and \( \beta \) are both either real or imaginary. In order to have real energy eigenvalues both \( \alpha \) and \( \beta \) have to be real, while to have complex bound state spectrum, i.e. in the case of spontaneous breakdown of \( PT \) symmetry one of them has to take an imaginary value [22]. If both \( \alpha \) and \( \beta \) are imaginary, then there are no bound states. Here we assume that \( \beta \) is real, and \( \alpha \) can be real or imaginary, depending on whether the \( PT \) symmetry is unbroken or broken. This choice does not restrict the generality of the problem, since the roles of \( \alpha \) and \( \beta \) can easily be reversed (see (21) in the Appendix).

For the Scarf II potential the breakdown of \( PT \) symmetry takes place when the strength of the imaginary potential component exceeds a certain limit depending on the strength of the real potential component, as described in Ref. [9]. This condition corresponds exactly to taking imaginary values for \( \alpha \) instead of real ones (see e.g. Ref. [22] for the details), so a smooth transition over the critical point can be achieved by moving \( \alpha \) to zero along the real axis and then continuing along the imaginary axis.
In the PT symmetric case there are two sets of normalizable solutions [6,17,18], which carry the upper indexes \((\alpha, \beta)\) and \((-\alpha, \beta)\) in (3). Obviously, (1) is not sensitive to the + or − sign of \(\alpha\). In the notation of Ref. [20] the two solutions corresponds to quasi-parity \(q = +1\) and \(-1\). This sign difference results in two distinct energy eigenvalues in (2), which form a complex conjugate pair when \(\alpha\) is imaginary, i.e. in the case of broken PT symmetry. In this case the PT operation transforms the two solutions into each other, while in the unbroken symmetry case the two solutions are eigenfunctions of the PT operator.

In the following sections we are going to evaluate integrals containing the standard and PT symmetric inner product of wavefunctions of the type \(\psi_n^{\pm \alpha, \beta}(x)\) (3). The technical details of the calculations can be found in the Appendix.

3 The PT symmetric inner product and the pseudo-norm

Let us consider the PT symmetric inner product [13,14] of two solutions of the type (3)

\[
I_{nl}^{(\alpha, \beta, \delta)} = \int_{-\infty}^{\infty} \psi_n^{(\alpha, \beta)}(x)\overline{\psi_l^{(\delta, \beta)}(-x)} dx .
\] (4)

According to our choice, \(\beta\) is real and \(\delta\) can be \(\pm \alpha\), depending on whether we calculate the PT symmetric inner product of states with the same or different quasi-parities (\(\delta = \alpha\) and \(\delta = -\alpha\), respectively), furthermore, \(\alpha\) can be real or imaginary, depending on whether the PT symmetry is unbroken or broken. Applying (21) and (22) presented in the Appendix, we can write

\[
I_{nl}^{(\alpha, \beta, \delta)} = C_n^{(\alpha, \beta)}[C_l^{(\delta, \beta)}]^*(-1)^nQ_{nl}^{(\alpha, \beta, \delta)} .
\] (5)

This formula together with (29) has significant implications regarding the PT symmetric inner product (4). First note that whenever \(\alpha = -\delta^*\) holds, the integral vanishes due to the presence of the \(\sin[\pi(\alpha + \delta^*)]\) term in (29). This corresponds to either \(\alpha = \delta\) with imaginary \(\alpha\), i.e. the inner product of wavefunctions of the same type (same quasi-parity) in the broken PT symmetry case, or \(\alpha = -\delta\) with real \(\alpha\), i.e. the inner product of two different type (different quasi-parity) wavefunctions in the unbroken PT symmetry case. So we can conclude that the two states are orthogonal in these situations.

Now let us consider the cases when \(\alpha \neq -\delta^*\). The first case is \(\delta = \alpha\) with real \(\alpha\) (unbroken PT symmetry). Substituting this \(\delta\) in (34) (and remembering that \(\beta\) is real) we get
\[ I_{nl}^{(\alpha,\beta,\alpha)} = \delta_{nl} |C_n^{(\alpha,\beta)}|^2 \frac{2^{\alpha+\beta+2}}{\alpha + \beta + 2n + 1} \frac{\sin(\pi \alpha) \sin(\pi \beta)}{\sin[\pi(\alpha + \beta)]} \times \left( \frac{\alpha + \beta + 2n}{n + \beta} \right)^{-1} \left( \frac{\alpha + \beta + 2}{n} \right). \]  

(6)

This proves directly the orthogonality of the states of the same type (i.e. those with the same quasi-parity) for \( n \neq l \) when the \( PT \) symmetry is unbroken, and gives a closed formula for the pseudonorm for \( n = l \). Previously this pseudonorm was known only for the ground state \( n = 0 \) [20], while the orthogonality of the eigenfunctions was proven only indirectly [14,9]. This latter proof rests on the equation

\[ (E_n - E_l^*) \int_{-\infty}^{\infty} \psi_n(x)\psi_l^*(-x)dx = 0 , \]  

(7)

which is the equivalent of the equation proving the real nature of the energy eigenvalues for Hermitian systems. In the case of unbroken \( PT \) symmetry \( E_n \) and \( E_l \) are real and they are not equal, consequently the integral in (7) has to vanish.

The only remaining case is \( \delta = -\alpha \) with imaginary \( \alpha \), when \( \delta^* = \alpha \) holds again. This case gives us the overlap of eigenstates belonging to different quasi-parity in the broken \( PT \) symmetry case. It turns out that the \( I_{nl}^{(\alpha,\beta,-\alpha)} \) overlap has the same form as (6), except that \( |C_n^{(\alpha,\beta)}|^2 \) has to be replaced with \( C_n^{(\alpha,\beta)}[C_l^{(-\alpha,\beta)}]^* \).

Let us summarize the results for the different cases.

- Unbroken \( PT \) symmetry (\( \alpha \) real), same type wavefunctions: \( I_{nl}^{(\alpha,\beta,\alpha)} \) is diagonal in \( n \) and \( l \), as seen from Eq. (6). To extract more information, we can rewrite Eq. (6) in a somewhat different form, after eliminating the sine functions from the formulas by combining them with some gamma functions via \( \Gamma(x)\Gamma(1-x) = \pi/\sin \pi x \):

\[ I_{nl}^{(\alpha,\beta,\alpha)} = \delta_{nl} (-1)^n \pi |C_n^{(\alpha,\beta)}|^2 \frac{2^{\alpha+\beta+2}}{(-\alpha - \beta - 2n - 1)n! \Gamma(-\alpha - n)\Gamma(-\beta - n)} \]  

(8)

Due to the condition for having bound states, i.e. \( n < -[\text{Re}(\alpha) + \beta + 1]/2 \), if \( \alpha \) is real, then in Eq. (8) every term is positive, except \((-1)^n\) which alternates, and \( [\Gamma(-\alpha - n)\Gamma(-\beta - n)]^{-1} \), which is real, but its sign depends on the relative magnitude of \( \alpha, \beta \) and \( n \). Except for extreme values of \( \alpha \) and \( \beta \) the argument of the two gamma functions is positive for the first few \( n \)'s, so then the alternating \((-1)^n\) factor determines the sign of the pseudonorm, but as \( n \) reaches \(-\alpha \) and/or \(-\beta \), this regular pattern changes. The results of this case are new, except for \( n = 0 \).
• Unbroken $PT$ symmetry ($\alpha$ real), different type wavefunctions: $I_{nl}^{(\alpha,\beta,-\alpha)} = 0$, due to $\sin \pi(\alpha - \alpha^*) = 0$ in (29). This was proven indirectly by (7) [14,9].

• Broken $PT$ symmetry ($\alpha$ imaginary), same type wavefunctions: $I_{nl}^{(\alpha,\beta,\alpha)} = 0$, due to $\sin \pi(\alpha - \alpha^*) = 0$ in (29). This was proven indirectly by (7) [14,9].

• Broken $PT$ symmetry ($\alpha$ imaginary), different type wavefunctions: $I_{nl}^{(\alpha,\beta,-\alpha)}$ is diagonal in $n$ and $l$, as seen from Eq. (6). But in this case it seems that for $n = l$ there can be two different wavefunctions which are not orthogonal, in general. Equation (8) holds for this case too, except for a change in the term containing the normalization constants, as discussed before. This non-orthogonality of two different states is a new feature of $PT$ symmetric problems, which in this case appears only when the $PT$ symmetry is broken. This unusual result seems to be supported by Eq. (7): when the $PT$ symmetry is broken, the energies of the two states with the same principal quantum number $n$ but with different quasi-parity are complex conjugate to each other, so the zero value of (7) is secured by the energy term, and the integral need not be zero.

4 The Hermitian Scarf II potential and the normalization coefficients of the wavefunctions

As discussed in the Introduction, the normalization coefficients of the wavefunctions have not been determined as yet, due to the involved mathematics [21,9]. Here we use our new approach and show that it can also be applied to evaluate integrals for the conventional Scarf II potential.

Let us now denote the (standard) inner product of the states (3) as

$$K_{nl}^{(\alpha,\beta)} = \int_{-\infty}^{\infty} \psi_n^{(\alpha,\beta)}(x) \psi_l^{(\alpha,\beta)}(x)^* dx$$

(9)

Remember that in this case there is only one set of bound-state eigenfunctions, and that in this case we have $\alpha^* = \beta$. It is easy to show that

$$K_{nl}^{(\alpha,\beta)} = C_n^{(\alpha,\beta)} [C_l^{(\alpha,\beta)}]^* Q_{nl}^{(\alpha,\beta,\alpha,\beta)}.$$  

(10)

Note that $\delta^* = \alpha^* = \beta$ and $\gamma^* = \beta^* = \alpha$ holds now, so the conditions under which the general integral can be reduced to a simple form are again satisfied. The final result is rather similar to (8) obtained for the $PT$ symmetric case, except that the alternating $(-1)^n$ factor is now missing:

$$K_{nl}^{(\alpha,\beta)} = \delta_n \pi |C_n^{(\alpha,\beta)}|^2 \frac{2^{\alpha+\beta+2}}{(-\alpha - \beta - 2n - 1)n!} \frac{\Gamma(-\alpha - \beta - n)}{\Gamma(-\alpha - n)\Gamma(-\beta - n)}.$$  

(11)
It is easy to verify that this integral is always positive as it should. For this we recall that \( \alpha^* = \beta \), so \( \alpha + \beta \) is real. We also recall the condition for bound states \( n < -(\text{Re}[\alpha + \beta] + 1)/2 \), so the only terms which can introduce negative (and complex) quantities are the two gamma functions in the denominator. However, their product is now \( \Gamma(-\alpha - n)[\Gamma(-\alpha - n)]^* = |\Gamma(-\alpha - n)|^2 > 0 \), so we conclude that \( K_n^{(\alpha, \beta)} > 0 \). Equation (11) thus determines the normalization coefficients of the bound-state wavefunctions of the conventional Scarf II potential for the first time:

\[
C_n^{(\alpha, \beta)} = 2^{-\frac{\alpha + \beta}{2} - 1} \left[ \frac{\Gamma(-\alpha - n)\Gamma(-\beta - n)(-\alpha - \beta - 2n - 1)n!}{\Gamma(-\alpha - \beta - n)\pi} \right]^{1/2}.
\] (12)

5 The \( PT \) symmetric Scarf II potential as a conventional complex potential

As we have discussed in the Introduction, since the \( PT \) symmetric Scarf II potential is defined on the real \( x \) axis, it can also be considered as an ordinary complex potential, and the same overlap and normalization integrals can also be evaluated for it too. This means using the wavefunctions of the \( PT \) symmetric problem in inner products of the type (9). As expected for a complex potential, the states cease to be orthogonal, as it can be shown by direct calculation of integrals of the type (10) with real values of \( \beta \) and real or imaginary values of \( \alpha \). Technically this is reflected by the fact that the conditions \( \delta^* = \alpha \) and \( \gamma^* = \beta \), which were used in the Appendix to bring the sums to a closed form are not satisfied. However, some interesting results can be obtained calculating some diagonal matrix elements and overlaps.

Starting from the one-dimensional Schrödinger equation for a generic complex potential

\[
-\psi''(x) + [U(x) + iW(x)]\psi(x) = (E_R + iE_I)\psi(x)
\] (13)

for normalizable eigenfunctions \( \psi(x) \), we can derive [25,26] the following relation connecting the imaginary component of the potential and of the energy eigenvalue:

\[
\frac{\int_{-\infty}^{\infty} \psi(x)W(x)[\psi(x)]^*dx}{\int_{-\infty}^{\infty} \psi(x)[\psi(x)]^*dx} = E_I
\] (14)

This relation can be rather useful in demonstrating the \( PT \) symmetry breaking mechanism: tuning the potential parameters from the domain of unbroken
PT symmetry to the domain of symmetry breaking should result in the appearance of a non-zero value of $E_I$. For the Scarf II potential this means shifting $\alpha$ along the real axis up to zero, and then continuing along the imaginary axis.

Specifying (14) to (1) and (3), we get

$$G_n(\alpha, \beta) \equiv \frac{\int_{-\infty}^{\infty} \psi_n^{(\alpha, \beta)}(x) \frac{\beta^2 - \alpha^2}{2 \cosh^2 x} \sinh x \psi_n^{(\alpha, \beta)}(x)^* dx}{\int_{-\infty}^{\infty} \psi_n^{(\alpha, \beta)}(x) (\psi_n^{(\alpha, \beta)}(x))^* dx} \equiv \frac{J_n^{(\alpha, \beta)}}{J_n^{(\alpha, \beta)}}$$

for the integrals, where we assume that $\psi_n^{(\alpha, \beta)}(x)$ is a normalizable eigenfunction of the PT symmetric Scarf II potential, i.e. $\beta$ is real, and $\alpha$ is either real or imaginary, depending on whether the PT symmetry is unbroken or broken. The integral in the denominator can be expressed implicitly in a form similar to the diagonal version of Eq. (4):

$$L_n^{(\alpha, \beta)} = |G_n^{(\alpha, \beta)}|^2 2^{\frac{\alpha + \alpha^*}{2} + \beta + 2} \frac{\sin[\pi (\alpha^* + \beta)]/2 \sin[\pi (\alpha + \beta)]/2}{\sin[\pi (\beta + (\alpha + \alpha^*)/2)]}$$

$$\times \sum_{m=0}^{n} (-1)^m \begin{pmatrix} n + \alpha \\ m \end{pmatrix} \begin{pmatrix} n + \beta \\ n - m \end{pmatrix} \sum_{m'=0}^{n} (-1)^{m'} \begin{pmatrix} n + \alpha^* \\ m' \end{pmatrix} \begin{pmatrix} n + \beta \\ n - m' \end{pmatrix}$$

$$\times \frac{\Gamma(\frac{\alpha + \beta}{2} + n + 1 - m + m') \Gamma(\frac{\alpha^* + \beta}{2} + n + 1 + m - m')}{\Gamma(\frac{\alpha + \alpha^*}{2} + \beta + 2n + 2)}$$

This integral can also be expressed in terms of the $Q_n^{(\alpha, \beta, \gamma, \delta)}$ quantity (22). However, in this case we have $\gamma = \alpha$ and $\delta = \beta$, so the conditions (31) for reducing the implicit summed expression into a closed formula are not satisfied. Nevertheless, it is technically not too involved to evaluate (16) for the first few values of $n$.

A similar expression holds also for the integral appearing in the numerator, which can be brought to a sum form using (28):

$$J_n^{(\alpha, \beta)} = \frac{i}{2} (\beta^2 - \alpha^2) |G_n^{(\alpha, \beta)}|^2 2^{\frac{\alpha + \alpha^*}{2} + \beta} \frac{\sin[\pi (\alpha^* + \beta)]/2 \sin[\pi (\alpha + \beta)]/2}{\sin[\pi (\beta + (\alpha + \alpha^*)/2)]}$$

$$\times \sum_{m=0}^{n} (-1)^m \begin{pmatrix} n + \alpha \\ m \end{pmatrix} \begin{pmatrix} n + \beta \\ n - m \end{pmatrix}$$

$$\times \sum_{m'=0}^{n} (-1)^{m'} \begin{pmatrix} \alpha - \alpha^* \\ 2m - 2m' \end{pmatrix} \begin{pmatrix} n + \alpha^* \\ m' \end{pmatrix} \begin{pmatrix} n + \beta \\ n - m' \end{pmatrix}$$
\[
\frac{\Gamma\left(\frac{\alpha + \beta}{2} + n - m + m'\right)\Gamma\left(\frac{\alpha + \beta}{2} + n + m - m'\right)}{\Gamma\left(\frac{\alpha + \alpha^*}{2} + \beta + 2n\right)}.
\]

(17)

This expression can also be evaluated directly relatively easily for the first few values of \(n\). It also turns out that an \(\alpha - \alpha^*\) can be factored out from the integral (17).

From Eq. (2) we expect

\[
\text{Im}(E_n^{(\alpha,\beta)}) = \frac{i}{8}(\alpha - \alpha^*)(\alpha + \alpha^* + 2\beta + 4n + 2),
\]

and we indeed get this expression by direct calculation from (15), (16) and (17). This expression vanishes (as it should) for real values of \(\alpha\), i.e. for unbroken \(PT\) symmetry. When the symmetry is broken (\(\alpha\) is imaginary), then the second factor in (18) comes from the ratio of the gamma functions in the denominator of (17) and (16).

6 Summary

We have studied the Scarf II potential in its general form, which contains both its Hermitian and its \(PT\) symmetric version, depending on the choice of the potential parameters \(\alpha\) and \(\beta\). Our work was motivated by the fact that this potential is a perfect laboratory to test the peculiarities of \(PT\) symmetric quantum mechanics, and in particular, the mechanism of the breakdown of \(PT\) symmetry. This is because it has no singularities on the \(x\) axis.

The \(PT\) symmetric version of the Scarf II potential is obtained when \(\beta\) is chosen to be real, and \(\alpha\) real or imaginary, depending on whether the \(PT\) symmetry is broken or unbroken: in the former case the bound-state energy spectrum is completely real, while in the latter case it is fully complex. The reality of \(\beta\) is not an essential restriction, since the roles of \(\alpha\) and \(\beta\) can be interchanged in a trivial way. The potential is not sensitive to the sign of \(\alpha\), and this is reflected by the fact that both in the unbroken and broken \(PT\) symmetry case there are two sets of normalizable (bound) states with the same value of the principal quantum number \(n\), and they are distinguished by the sign of \(\alpha\), i.e. the quasi-parity. The corresponding energy eigenvalues are different: they are both real for unbroken \(PT\) symmetry, and they form a complex conjugate pair when the symmetry is broken.

We have devised a way by which the modified inner product of the wave-functions \(I_{nl}^{(\alpha,\beta,\pm\alpha)} \equiv \langle \psi_n^{(\alpha,\beta)} | P | \psi_l^{(\pm\alpha,\beta)} \rangle\) can be evaluated explicitly. We have shown that these states are orthogonal in \(n\) and in the quasi-parity quantum
numbers, except when $\alpha$ is imaginary, i.e. the $PT$ symmetry is broken, and
the inner product of two states with the same $n$ but different quasi-parities
is considered. We derived a closed expression for the diagonal inner products,
i.e. the pseudo-norm, and we found that its sign is indefinite, as expected from
more general considerations. However, the sign of the pseudo-norm depends
on $\alpha$ and $\beta$ in a rather complicated way, so no compact rule can be formulated
for its sign.

Using the same techniques we also determined the standard inner product
of the Hermitian Scarf II wavefunctions. In this case $\alpha^* = \beta$ holds, and there is
only one set of bound-state wavefunctions; the other one represents resonances:
both the orthogonality of the states, the normalization constants for the Scarf
II potential have been derived for the first time.

We also analysed the $PT$ symmetric Scarf II potential as an ordinary complex
potential. For this, we evaluated two types of diagonal matrix elements (using
the standard inner product) of the $PT$ symmetric wavefunctions: the matrix
element of the imaginary component of the potential and the norm. The ratio
of these gives a closed expression for the imaginaly component of the energy,
which contains the potential parameters and thus can be used to study the
breakdown of $PT$ symmetry as the value of $\alpha$ is tuned from real values to
imaginary ones through 0. In the case of other solvable $PT$ symmetric poten-
tials this transition requires crossing a singular point of the potential, which
obscures important aspects of $PT$ symmetry breaking.

**Acknowledgment**

This work was supported by the OTKA grant No. T031945 (Hungary), INFN
and ENEA (Italy).

**Appendix**

Here we derive a general formula for the integrals which includes as special
cases both the Hermitian and the $PT$ symmetric inner product of the wave-
functions.

First, let’s define the functions

$$ F_n^{(\alpha,\beta)}(x) = (1 - i \sinh(x))^{\frac{\alpha}{2} + \frac{1}{4}} (1 + i \sinh(x))^{\frac{\beta}{2} + \frac{1}{4}} P_n^{(\alpha,\beta)}(i \sinh(x)) , \quad (19) $$
which are the bound-state Scarf II wavefunctions (3) without the normalization constant. The Jacobi polynomials appearing in (19) take the form [23]

\[ P_n^{(\alpha,\beta)}(i \sinh(x)) = \frac{1}{2^n} \sum_{m=0}^{n} \binom{n + \alpha}{m} \binom{n + \beta}{n - m} \times (-1)^{n-m} (1 - i \sinh(x))^{n-m}(1 + i \sinh(x))^m. \]  

Also due to the properties of the Jacobi polynomials [23] the (19) functions transform under spatial reflection (i.e. the $P$ operation) in the following way:

\[ F_n^{(\alpha,\beta)}(-x) = (1 + i \sinh(x))^{\frac{\alpha}{2} + \frac{1}{4}} (1 - i \sinh(x))^{\frac{\beta}{2} + \frac{1}{4}} F_n^{(\alpha,\beta)}(-i \sinh(x)) \]

\[ = (-1)^n (1 - i \sinh(x))^{\frac{n+\beta+1}{4}} (1 + i \sinh(x))^{\frac{n+\alpha+1}{4}} P_n^{(\beta,\alpha)}(i \sinh(x)) \]

\[ = (-1)^n F_n^{(\beta,\alpha)}(x) \]  

(21)

Now define the integral

\[ Q_{nl}^{(\alpha,\beta,\gamma,\delta)} = \int_{-\infty}^{\infty} F_n^{(\alpha,\beta)}(x) [F_l^{(\gamma,\delta)}(x)]^* dx. \]

(22)

This integral contains the formulae necessary to evaluate the standard (Hermitian) inner product of the ordinary (real) Scarf II bound-state eigenfunctions (with $\gamma = \alpha$ and $\delta = \beta$) and the $PT$ symmetric inner product of the eigenfunctions of the $PT$ symmetric Scarf potential with equal and different quasi-parity (with $\gamma = \beta$, $\delta = \alpha$ and $-\alpha$, respectively). Note that in the latter case the roles of $\gamma$ and $\delta$ are interchanged, due to (21). The above formula can also be used, of course, to evaluate integrals appearing in the Hermitian inner product of the eigenfunctions of the $PT$ symmetric Scarf II potential, however, we shall find that in this case it cannot be reduced to simpler forms.

First we need to evaluate integrals of the kind

\[ A_{0}^{(p,q)} \equiv \int_{-\infty}^{\infty} (1 - i \sinh x)^p (1 + i \sinh x)^q dx, \]

(23)

which then appear in sums in (22). The integral can then be evaluated in a multistep procedure [20,27]:

\[ A_{0}^{(p,q)} = \int_{-\infty}^{\infty} \cosh^{p+q} x \exp[(q - p) \tanh^{-1}(i \sinh x)] \]

(24)
\[= \int_{-\infty}^{\infty} \cosh^{p+q} x \exp[i(q-p) \tan^{-1}(\sinh x)] \quad (25)\]

\[= \int_{-\pi/2}^{\pi/2} \cos^{-(p+q+1)} y \exp[i(q-p)y] \quad (26)\]

\[= 2^{p+q+1} \pi \frac{\Gamma(-q)}{\Gamma(-p+1/2)\Gamma(-q+1/2)}. \quad (27)\]

In (24) we applied the relation \(\tanh^{-1} z = \frac{1}{2} \ln \frac{1+z}{1-z}\) which is also used sometimes to write the Scarf II wavefunctions in an alternative form [21,9,20], and in (26) a change of variables was performed: \(\tan y = \sinh x\). This method was used in Ref. [20] to evaluate the pseudo-norm of the ground-state wavefunctions for unbroken \(PT\) symmetry. In what follows we shall also find it useful to evaluate another integral, which follows directly from (27):

\[A_1^{(p,q)} \equiv \int_{-\infty}^{\infty} \sinh x (1-i \sinh x)^p (1+i \sinh x)^q dx = i^{p-q} \frac{p+q+1}{p+q+1} A_0^{(p,q)}. \quad (28)\]

In the next step we have to evaluate sums of integrals of the type (23) appearing in (22):

\[Q_{nl}^{(\alpha,\beta,\gamma,\delta)} = (-1)^{n+l} 2^{\frac{\alpha+\beta+\gamma^*+\delta^*}{2}+2} \frac{\sin[\pi(\alpha+\delta^*)/2] \sin[\pi(\beta+\gamma^*)]}{\sin[\pi(\alpha+\beta+\gamma^*+\delta^*)/2]} \times \sum_{m=0}^{n} (-1)^m \binom{n+\alpha}{m} \binom{n+\beta}{n-m} \sum_{m'=0}^{l} (-1)^{m'} \binom{l+\gamma^*}{m'} \binom{l+\delta^*}{l-m'} \times \frac{\Gamma\left(\frac{\alpha+\delta^*}{2}+n-m+m'+1\right) \Gamma\left(\frac{\beta+\gamma^*}{2}+l+m-m'+1\right)}{\Gamma\left(\frac{\alpha+\beta+\gamma^*+\delta^*}{2}+n+l+2\right)}. \quad (29)\]

Without the loss of generality we can assume that \(n \leq l\). With some rearrangement of the binomial coefficient and the gamma functions we can rewrite the last sum (over \(m'\)) into

\[\frac{\Gamma(l+\gamma^*+1) \Gamma(l+\delta^*)}{\Gamma\left(\frac{\alpha+\beta+\gamma^*+\delta^*}{2}+n+l+1\right) l!} \sum_{m'=0}^{l} (-1)^{m'} \binom{l}{m'} \times \frac{\Gamma\left(\frac{\alpha+\delta^*}{2}+n-m+m'+1\right) \Gamma\left(\frac{\beta+\gamma^*}{2}+l+m-m'+1\right)}{\Gamma\left(\gamma^*+l-m'+1\right) \Gamma\left(\delta^*+m'+1\right)}. \quad (30)\]

In what follows we assume that the relations

\[\delta^* = \alpha \quad \gamma^* = \beta \quad (31)\]
hold, in order to bring (30) to a simpler form. This assumption turns out to be valid for the most important cases, as it is described in the appropriate sections. Under the conditions (31) the two terms containing the ratios of gamma functions in (30) can be written as a finite power series of $m'$: 
\[ \sum_{j=0}^{n} c_j (m')^j. \]
This clearly follows from the two ratios of the gamma functions: the first one contains $m'$ up to the $(n - m)$'th power in the form \((\alpha + m' + 1)(\alpha + m' + 2) \cdots (\alpha + m' + n - m)\), while the second one contains it up to the $m'$th power as \((\beta + l - m' + 1)(\beta + l - m' + 2) \cdots (\beta + l - m' + m)\).

Now observing Eqs. 4.2.2.3 and 4.2.2.4 of Ref. [27] we find that
\[
\sum_{m'=0}^{l} (-1)^{m'} \left( \begin{array}{c} l \\ m' \end{array} \right) \sum_{j=0}^{n} c_j (m')^j = \sum_{j=0}^{n} c_j \sum_{m'=0}^{l} (-1)^{m'} \left( \begin{array}{c} l \\ m' \end{array} \right) (m')^j = \sum_{j=0}^{n} c_j \delta_{jl} (-1)^{l!} (32)
\]

Since we assumed that $n \leq l$ holds, $j \leq l$ is also valid, so this sum can be non-zero only for $n = l$. In this case its value is
\[
\delta_{ln} (-1)^n n! c_n = \delta_{ln} (-1)^n n! (-1)^m = \delta_{ln} n! (-1)^{n+m}. (33)
\]

Here we used that $c_n$, the coefficient of $(m')^n$ (the highest possible power of $m'$) in the power series is $(+1)^{n-m} (-1)^m$, as can be seen from the factorization of the ratio of the gamma functions above. Substituting this result into (30) and (29) and then using Eq. 4.2.5.19 of Ref. [27], we get
\[
Q_{nl}^{(\alpha, \beta, \gamma, \delta=\alpha^*)} = \delta_{nl} (-1)^n \frac{2^{\alpha+\beta+2}}{\alpha + \beta + 2n + 1} \sin(\pi \alpha) \sin(\pi \beta) \sin[\pi(\alpha + \beta)] \\
\times \left( \begin{array}{c} \alpha + \beta + 2n \\ n + \beta \end{array} \right)^{-1} \left( \begin{array}{c} \alpha + \beta + 2n \\ n \end{array} \right). (34)
\]

Finally, we note that for the $n = l$ diagonal case (29) can be evaluated in an alternative way too, using the sum rule
\[
\sum_{k=0}^{n} (-1)^k \left( \begin{array}{c} n \\ k \end{array} \right) \left( \begin{array}{c} a - m - k \\ n - m \end{array} \right) \left( \begin{array}{c} b + m + k \\ m \end{array} \right) = (-1)^m \left( \begin{array}{c} n \\ m \end{array} \right). (35)
\]

The interesting feature of this result is that the right hand side is independent of $a$ and $b$. This formula is missing from the standard compilation [27], and
can be proven by an induction in \( n \), using also the properties of the binomial coefficients.

**References**

[1] C. M. Bender, S. Boettcher, Phys. Rev. Lett. 24 (1998) 5243; J. Phys. A 31 (1998) L273.

[2] C. M. Bender, S. Boettcher, P. N. Meisinger, J. Math. Phys. 40 (1999) 2201.

[3] F. M. Fernández, R. Guardiola, J. Ros, M. Znojil, J. Phys. A 31 (1998) 3105; C. M. Bender, G. V. Dunne, P. N. Meisinger, Phys. Lett. A 252 (1999) 272; M. Znojil, J. Phys. A 32 (1999) 7419.

[4] F. M. Fernández, R. Guardiola, J. Ros, M. Znojil, J. Phys. A 31 (1998) 10105; E. Caliceti, S. Graffi, M. Maioli, Commun. Math. Phys. 75 (1980) 51; C. M. Bender, G. V. Dunne, J. Math. Phys. 40 (1999) 4616.

[5] M. Znojil, Phys. Lett. A 259 (1999) 220; J. Phys. A 33 (2000) 4561; J. Phys. A 33 (2000) L61; J. Phys. A 34 (2001) 9585.

[6] G. Lévai, M. Znojil, J. Phys. A 33 (2000) 7165.

[7] B. Bagchi, R. Roychoudhury, J. Phys. A 33 (2000) L1; F. Cannata, M. Ioffe, R. Roychoudhury, P. Roy, Phys. Lett. A 281 (2001) 305.

[8] F. Cannata, G. Junker, J. Trost, Phys. Lett. A 246 (1998) 219; B. Bagchi, S. Mallik, C. Quesne, Int. J. Mod. Phys. A 17 (2002) 51.

[9] Z. Ahmed, Phys. Lett. A 282 (2001) 343.

[10] M. Znojil, G. Lévai, Mod. Phys. Lett. A 16 (2001) 2273.

[11] A. Khare, B. P. Mandal, Phys. Lett. A 272 (2000) 53.

[12] C. M. Bender, F. Cooper, P. N. Meisinger, V. M. Savage, Phys. Lett. A 259 (1999) 224.

[13] M. Znojil, [quant-ph/0103054](http://arxiv.org/abs/quant-ph/0103054) v3, 30 Oct. 2001.

[14] G. S. Japaridze, J. Phys. A 35 (2002) 1709.
[15] L. E. Gendenshtein, Zh. Eksp. Teor. Fiz. Pis. Red. 38 (1983) 299 (Eng. transl. JETP Lett. 38 (1983) 35).

[16] Z. Ahmed, Phys. Lett. A 290 (2001) 19.

[17] B. Bagchi, C. Quesne, Phys. Lett. A 273 (2000) 285.

[18] G. Lévai, F. Cannata and A. Ventura, J. Phys. A 34 (2001) 839.

[19] G. Lévai, F. Cannata and A. Ventura, submitted.

[20] B. Bagchi, C. Quesne and M. Znojil, Mod. Phys. Lett. A 16 (2001) 2047.

[21] J. W. Dabrowska, A. Khare, U. P. Sukhatme, J. Phys. A 21 (1988) L195.

[22] G. Lévai, M. Znojil, Mod. Phys. Lett. A 16 (2001) 1973.

[23] M. Abramowitz, I. A. Stegun, Handbook of Mathematical Functions, New York, Dover, 1970.

[24] G. Lévai, J. Phys. A 22 (1989) 689.

[25] D. Baye, G. Lévai, J.-M. Sparenberg, Nucl. Phys. A 599 (1996) 435.

[26] A. A. Andrianov, M. V. Ioffe, F. Cannata, J. P. Dedonder, Int. J. Mod. Phys. A 14 (1999) 2675.

[27] A. P. Prudnikov, Yu. A. Brychkov, O. I. Marichev, Integrals and Series, vol 1, Gordon And Breach, New York 1986.