

ON THE COMMON LIMIT OF THE \mathcal{PT} -SYMMETRIC ROSEN–MORSE II AND FINITE SQUARE WELL POTENTIALS

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ABSTRACT. Two \mathcal{PT} -symmetric potentials are compared, which possess asymptotically finite imaginary components: the \mathcal{PT} -symmetric Rosen–Morse II and the finite \mathcal{PT} -symmetric square well potentials. Despite their different mathematical structure, their shape is rather similar, and this fact leads to similarities in their physical characteristics. Their bound-state energy spectrum was found to be purely real, and this finding was attributed to their asymptotically non-vanishing imaginary potential components. Here the $V(x) = \gamma\delta(x) + i2\Lambda \operatorname{sgn}(x)$ potential is discussed, which can be obtained as the common limit of the two other potentials. The energy spectrum, the bound-state wave functions and the transmission and reflection coefficients are studied in the respective limits, and the results are compared.

KEYWORDS: \mathcal{PT} -symmetric potential; bound states; scattering; Dirac- δ limit.

1. INTRODUCTION

The introduction of \mathcal{PT} -symmetric quantum mechanics [1] gave strong impetus to the investigation of non-hermitian quantum mechanical systems (for a review, see [2]). In most cases these systems represent one-dimensional complex potentials that are invariant with respect simultaneous space (\mathcal{P}) and time (\mathcal{T}) reflection, where the latter corresponds to complex conjugation. Although these potentials are manifestly non-hermitian, they possess several features that are characteristic of hermitian systems, i.e. real potentials. Perhaps the most spectacular one among these is that their discrete energy spectrum is partly or completely real. This feature was first attributed to \mathcal{PT} symmetry, but later it soon turned out that \mathcal{PT} symmetry is neither a necessary, nor a sufficient condition for the presence of real energy eigenvalues. It was found that in many such systems the energy eigenvalues merge pairwise with increasing non-hermiticity, and reappear as complex conjugate pairs. Since at the same time the energy eigenstates cease to be eigenfunctions of the \mathcal{PT} operator, this phenomenon was interpreted as the breakdown of \mathcal{PT} symmetry. It was shown that from the mathematical point of view \mathcal{PT} symmetry is a particular case of pseudo-hermiticity [3]. More recently, after a decade of theoretical investigations the existence of \mathcal{PT} symmetry, as well as that of its breakdown was verified in quantum optical experiments [4].

Although the first \mathcal{PT} -symmetric potentials were solved by numerical methods, it was soon realized that most exactly solvable potentials can be cast into a \mathcal{PT} -symmetric form, and the usual techniques applied to their hermitian version can be used in the \mathcal{PT} -symmetric setting too (see [5–7] for reviews). The

\mathcal{PT} -symmetrization of shape-invariant [5, 6, 8] and of the more general Natanzon-class potentials [7] that are solved in terms of the (confluent) hypergeometric function [9] revealed that the characteristic features of \mathcal{PT} -symmetric potentials can conveniently be studied using the exact analytical solutions of these potentials.

A particularly interesting issue was the study of the breakdown of \mathcal{PT} symmetry: the transition through the critical point could be reached by fine tuning of some potential parameter, and the whole process could be kept under control. It was found that there are exactly solvable potentials that do not exhibit this feature [10–13], while some others do [14–18]. It was also noticed that in most cases the complexification of the energy eigenvalues occurs at the same value of the control parameter (sudden mechanism) [15–17], while in some cases it is a continuous process [18]. Although there are examples for this latter, gradual mechanism among Natanzon-class potentials [18], it seems to be characteristic of potentials not belonging to the Natanzon (and thus, the shape-invariant) class. Examples are the numerically solvable Bender-Boettcher potentials [1], some piecewise constant potentials, like the \mathcal{PT} -symmetric infinite square well [19], and the \mathcal{PT} -symmetric exponential potential [20].

The asymptotic behaviour of the imaginary potential component was found to play an important role in determining the characteristics of the energy spectrum. The \mathcal{PT} -symmetric Scarf II and Rosen–Morse II potentials share the same real component, $\cosh^{-2}(x)$, while their imaginary components are different. In the case of the Scarf II potential the imaginary potential component vanishes asymptotically, while in the case of the Rosen–Morse II potential it is the $i \tanh(x)$ function, reaching finite values for $x \rightarrow \pm\infty$.

In the former case the breakdown of \mathcal{PT} symmetry can occur [15], while in the latter the discrete energy spectrum is purely real [10]. This latter finding was later proven for all three PII-class shape-invariant potentials (Rosen–Morse I, II, Eckart) using a thorough analysis of \mathcal{PT} -symmetric Natanzon-class potentials [7]. This clear difference can obviously be attributed to the different asymptotic behaviour of the two potentials [21].

This peculiar character of the asymptotically constant imaginary potential component characterising the \mathcal{PT} -symmetric Rosen–Morse II potential inspired the investigation of further potentials with similar structure. A natural candidate was the finite \mathcal{PT} -symmetric square well potential [22], which is essentially the finite real square well potential supplemented outside the well by a constant imaginary component with opposite sign on the two sides. In a way, this potential can be considered an approximation of the \mathcal{PT} -symmetric Rosen–Morse II potential: the $\cosh^{-2}(x)$ and $i \tanh(x)$ terms are mimicked by the finite real square well and the constant imaginary terms, respectively. It was supposed [22] that given the similar shapes, the main physical features of the two potentials would also be close to each other. It was found that the energy spectrum of the finite \mathcal{PT} -symmetric square well potential is purely real, similarly to that of the \mathcal{PT} -symmetric Rosen–Morse II potential. Another similarity was that by increasing non-hermiticity, i.e. the coupling coefficient of the imaginary potential component, the energy eigenvalues are rapidly lifted to the positive domain $E > 0$. There was, however, an important difference: while the number of bound states was fixed for the Rosen–Morse II potential, it was infinite for the finite \mathcal{PT} -symmetric square well potential. The additional states were found to be the equivalents of transmission resonances of the real finite square well potential [22].

These results naturally inspire further investigation of \mathcal{PT} -symmetric potentials with asymptotically constant imaginary component. Here a potential of this kind is investigated, which, furthermore, can be obtained as the common limit of the \mathcal{PT} -symmetric versions of the Rosen–Morse II and finite square well potentials:

$$V(x) = \gamma\delta(x) + i2\Lambda \operatorname{sgn} x. \quad (1)$$

The purpose of this work is to explore how the physical quantities of the \mathcal{PT} -symmetric Rosen–Morse II and finite square well potentials behave when the limit as above is implemented.

The paper is organized as follows. Sections 2 and 3 discuss the specific limits of the \mathcal{PT} -symmetric Rosen–Morse II and finite square well potentials, respectively. In Section 4 the results are summarized and are compared with those obtained for other potentials with various asymptotic behaviour.

2. THE \mathcal{PT} -SYMMETRIC ROSEN–MORSE II POTENTIAL

Let us consider the potential

$$V(x) = -\frac{s(s+1)a^2}{\cosh^2(ax)} + 2i\lambda a^2 \tanh(ax). \quad (2)$$

Noting that the $s \rightarrow -s - 1$ replacement leaves $V(x)$ invariant, we may choose $s \geq -1/2$. Following the discussion of [10] with the difference that x is rescaled by the positive real constant a as ax , the bound-state eigenvalues are

$$E_n = -a^2(s-n)^2 + \frac{\lambda^2 a^2}{(s-n)^2}, \quad (3)$$

while the corresponding wave functions are expressed in terms of Jacobi polynomials [23]

$$\psi_n(x) = C_n(1 - \tanh(ax))^{\frac{\alpha}{2}} \times (1 + \tanh(ax))^{\frac{\beta}{2}} P_n^{(\alpha, \beta)}(\tanh(ax)). \quad (4)$$

Here C_n is the normalization constant

$$C_n = \frac{i^n 2^{n-s}}{|\Gamma(s+1 + i\lambda/(s-n))|} \times \left(\frac{an! \Gamma(2s-n+1) ((s-n)^2 + \lambda^2/(s-n)^2)}{s-n} \right)^{1/2} \quad (5)$$

while

$$\alpha_n = s - n + \frac{i\lambda}{s-n}, \quad \beta_n = s - n - \frac{i\lambda}{s-n}. \quad (6)$$

It was shown in [10] that the number of bound states is always finite, and the upper limit does not depend on the parameter λ :

$$n < s. \quad (7)$$

It may be noted that for $-1 \leq s \leq 0$ the real component of (2) turns into a barrier with $V_{\max}(x) \leq a^2/4$, and there are no bound states in this case.

Let us reparametrize the potential in the following way:

$$\gamma = -2as(s+1), \quad \Lambda = a^2\lambda. \quad (8)$$

Considering then the following limits:

$$\delta(x) = \lim_{a \rightarrow \infty} \frac{a}{2 \cosh^2(ax)} \quad (9)$$

and

$$\operatorname{sgn}(x) = \lim_{a \rightarrow \infty} \tanh(ax). \quad (10)$$

the potential in (2) can be transformed into

$$V(x) = \gamma\delta(x) + 2i\Lambda \operatorname{sgn}(x). \quad (11)$$

Let us now clarify the effect of this limit on the energy eigenvalues (3) and wave functions (4). From (8) it follows that

$$s = -\frac{1}{2}(1 - (1 - 2\gamma/a)^{1/2}), \quad (12)$$

where the “-” sign inside the square brackets follows from the requirement $s > 0$. s can be expressed in a series involving the powers of $1/a$ as

$$s = -\frac{\gamma}{2a} - \frac{\gamma^2}{4a^2} + \mathcal{O}(a^{-3}). \quad (13)$$

Note that for $s > 0$ (8) implies that $\gamma < 0$. Recalling (7) this result also leads to the finding that only the ground state remains normalizable. Substituting s from (13) and Λ from (8) one finds that in the $a \rightarrow \infty$ limit the ground-state eigenvalue becomes

$$E_0 = -\frac{\gamma^2}{4} + \frac{4\Lambda^2}{\gamma^2}. \quad (14)$$

The corresponding wave function can be calculated after substituting s from (13) and Λ from (8) and $n = 0$ into (4) and (5), and taking the $a \rightarrow \infty$ limit:

$$\psi_0(x) = \begin{cases} C_0 \exp(-\kappa_+ x), & x > 0, \\ C_0 \exp(-\kappa_- x), & x < 0, \end{cases} \quad (15)$$

where

$$\kappa_{\pm} = -ik_{\pm} \pm \frac{\gamma}{2} - i\frac{2\Lambda}{\gamma}, \quad (16)$$

and

$$C_0 = \left(-\frac{2}{\gamma} \left(\frac{\gamma^2}{4} + \frac{4\Lambda^2}{\gamma^2} \right) \right)^{1/2}. \quad (17)$$

It can be seen that (15) satisfies \mathcal{PT} symmetry, i.e. $\mathcal{PT}\psi_0(x) = \psi_0^*(-x) = \psi_0(x)$. It is also found that

$$E_0 = -\kappa_{\pm}^2 \pm 2i\Lambda, \quad (18)$$

as expected. It is seen that the $i\text{sgn}(x)$ potential alone cannot support any bound state, rather the Dirac delta is also required for it. This is similar to the case of the \mathcal{PT} -symmetric Rosen–Morse II potential [10]: there the imaginary $2i\Lambda \tanh(ax)$ potential cannot support bound states without the presence of the real $-s(s+1)a^2/\cosh^2(ax)$ potential component.

It is worthwhile to check some special cases against already known results. For $\Lambda = 1/2$ the potential in (11) reduces to the one considered in [24], and (14) confirms the result $E_0 = -\gamma^2/4 + 1/\gamma^2$ discussed there. Furthermore, the $\Lambda = 0$ choice recovers the simple Dirac delta potential [25].

Finally, the hermitian case with a real step function can also be considered after replacing $\Lambda \rightarrow \pm i\Lambda$. In this case κ_{\pm} in (16) become real, and a bound state can appear only for

$$\frac{\gamma}{2} + \frac{2|\Lambda|}{\gamma} < 0, \quad (19)$$

i.e. for a negative γ satisfying $\gamma < -2(|\Lambda|)^{1/2}$.

The single real energy eigenvalue can also be obtained from the transmission coefficient. Adapting

the corresponding formulas from [10] one obtains for an incoming wave from the left

$$T_{L \rightarrow R} = \frac{-i\frac{k_-}{a}}{-s - i\frac{k_-}{2a} - i\frac{k_+}{2a}} \times \frac{\Gamma(1 - i\frac{k_-}{2a} - i\frac{k_+}{2a} - s)\Gamma(1 - i\frac{k_-}{2a} - i\frac{k_+}{2a} + s)}{\Gamma(1 - i\frac{k_+}{a})\Gamma(1 - i\frac{k_-}{a})} \quad (20)$$

and

$$R_{L \rightarrow R} = T_{L \rightarrow R} \frac{-s + i\frac{k_-}{2a} - i\frac{k_+}{2a}}{i\frac{k_-}{a}} \times \frac{\Gamma(1 - i\frac{k_+}{a})\Gamma(1 + i\frac{k_-}{a})}{\Gamma(1 + i\frac{k_-}{2a} - i\frac{k_+}{2a} - s)\Gamma(1 + i\frac{k_-}{2a} - i\frac{k_+}{2a} + s)}, \quad (21)$$

where

$$k_{\pm}^2 = E \mp 2i\Lambda \quad (22)$$

are the squared wave numbers obtained from the asymptotic limits $x \rightarrow \infty$ and $x \rightarrow -\infty$, respectively. For the sake of consistency the original notation k and k' was replaced by k_- and k_+ , and an error in the sign of k' was corrected in [10, eqs. (38)–(41)].

Recalling (13) and taking the $a \rightarrow \infty$ limit the terms with the gamma functions reduce to unity, so (20) and (21) turn into

$$T_{L \rightarrow R}(k_-, k_+) = \frac{2ik_-}{ik_- + ik_+ - \gamma} \quad (23)$$

and

$$R_{L \rightarrow R}(k_-, k_+) = \frac{ik_- - ik_+ + \gamma}{ik_- + ik_+ - \gamma}. \quad (24)$$

The transmission and reflection coefficients for the reverse direction are obtained by the $k_- \leftrightarrow k_+$ replacement. It is found that $T_{R \rightarrow L}(k_-, k_+) = T_{L \rightarrow R}(k_-, k_+)k_+/k_-$, so the difference is represented by a phase factor (as can be seen from (22)), while the reflection coefficients are related by $R_{R \rightarrow L}(k_-, k_+) = R_{L \rightarrow R}(k_-, k_+)(k_+ - k_- - i\gamma)/(k_- - k_+ - i\gamma)$. This handedness effect is similar to that observed for the \mathcal{PT} -symmetric Rosen–Morse II potential [10]. Note that in the case of asymptotically vanishing \mathcal{PT} -symmetric potentials the two transmission coefficients are strictly identical [26, 27].

The connection of the transmission and reflection coefficients to the bound state (15) will be discussed in Section 3, together with the corresponding results obtained there.

3. THE FINITE \mathcal{PT} -SYMMETRIC SQUARE WELL POTENTIAL

Let us consider the potential

$$V(x) = \begin{cases} -iv, & x < -\epsilon, \\ -V_0, & |x| < \epsilon, \\ iv, & x > \epsilon, \end{cases} \quad (25)$$

where ϵ and V_0 take on positive real values, and v takes on real value. For the case $v = 0$ potential (25) reduces to the real square well potential [28]. The sign of v is not significant, because changing the sign of v is practically equivalent with a spatial reflection, i.e. with the \mathcal{P} operation.

Following the discussion of [22] and using $2m = \hbar = 1$ units the solution of the time-independent Schrödinger equation can be described as

$$\psi(x) = \begin{cases} F^-(p_-)e^{ip_-x} + F^-(-p_-)e^{-ip_-x}, & x < -\epsilon, \\ \alpha \cos(kx) + i\beta \sin(kx), & |x| < \epsilon, \\ F^+(p_+)e^{ip_+x} + F^+(-p_+)e^{-ip_+x}, & x > \epsilon, \end{cases} \quad (26)$$

where

$$p_{\pm} = (E \mp iv)^{1/2}, \quad k = (E + V_0)^{1/2}. \quad (27)$$

E denotes the energy eigenvalue and the complex square root function is understood as in [23]. Note that in this case $[p_{\pm}]^* = p_{\mp}$ holds. The coefficients $F^-(p_-)$ and $F^+(p_+)$ can be determined from matching the solutions at $x = \pm\epsilon$ as

$$F^-(p_-) = \frac{1}{2ip_-} e^{ip_- \epsilon} ((\alpha p_- + \beta k)i \cos(k\epsilon) + (\alpha k + \beta p_-) \sin(k\epsilon)), \quad (28)$$

$$F^+(p_+) = \frac{1}{2ip_+} e^{-ip_+ \epsilon} ((\alpha p_+ + \beta k)i \cos(k\epsilon) - (\alpha k + \beta p_+) \sin(k\epsilon)), \quad (29)$$

while $F^-(-p_-)$ and $F^+(-p_+)$ follow from (28) and (29) by changing the sign of p_- and p_+ . Considering the case $v < 0$, following [22] the energy eigenvalues correspond to solutions that vanish asymptotically in both directions are searched as roots of equation

$$2kp_{+I} \cos(2k\epsilon) + (p_{+R}^2 + p_{+I}^2 - k^2) \sin(2k\epsilon) = 0 \quad (30)$$

on the real axis, where p_{+R} and p_{+I} are defined as the real and imaginary part of p_+ , i. e. $p_+ = p_{+R} + ip_{+I}$. Note that (30) establishes a connection between p_{+R} and p_{+I} when E is real. Taking into consideration (27) and separating the real and imaginary components of it, it turns out that the latter occurs only in the second term in the form $-i(v + 2p_{+R}p_{+I}) \sin(2k\epsilon)$. Since this expression has to be zero in general (irrespective of ϵ), it follows that

$$p_{+R} = -\frac{v}{2p_{+I}}. \quad (31)$$

To reproduce (11) let us reparametrize the potential (25) by introducing

$$\gamma = -2\epsilon V_0, \quad \Lambda = \frac{v}{2}. \quad (32)$$

Then keeping γ fixed and considering the $\epsilon \rightarrow 0$ limit the potential in (25) can be transformed into

$$V(x) = \gamma \delta(x) + 2i\Lambda \operatorname{sgn}(x) \quad (33)$$

as well.

In this limit, after applying the l'Hospital rule, equation (30) transform into $2p_{+I} + \gamma = 0$. Together with (31) and (32) this means that there is a single bound state with

$$p_{\pm} = \frac{2\Lambda}{\gamma} \mp i\frac{\gamma}{2}, \quad (34)$$

with the energy eigenvalue

$$E_0 = -\frac{\gamma^2}{4} + \frac{4\Lambda^2}{\gamma^2}, \quad (35)$$

which coincides with (14).

The transmission and reflection coefficients can be obtained from the corresponding limit of those in [22]. These coefficient for an incoming wave from the left are given by

$$T_{L \rightarrow R} = \frac{2ip_- k e^{-ip_- \epsilon} e^{-ip_+ \epsilon}}{ik \cos(2k\epsilon)(p_+ + p_-) + \sin(2k\epsilon)(p_+ p_- + k^2)} \quad (36)$$

and

$$R_{L \rightarrow R} = e^{-2ip_- \epsilon} \times \frac{ik(p_- - p_+) \cos(2k\epsilon) + (p_+ p_- - k^2) \sin(2k\epsilon)}{ik(p_+ + p_-) \cos(2k\epsilon) + (p_+ p_- + k^2) \sin(2k\epsilon)}, \quad (37)$$

respectively. In the $\epsilon \rightarrow 0$ limit they turn into

$$T_{L \rightarrow R} = \frac{2ip_-}{ip_- + ip_+ - \gamma} \quad (38)$$

and

$$R_{L \rightarrow R} = \frac{ip_- - ip_+ + \gamma}{ip_- + ip_+ - \gamma}, \quad (39)$$

respectively. The equivalent coefficients for a wave incoming from the right are obtained by the $p_+ \leftrightarrow p_-$ change, similarly to the results of Section 2.

Note that \mathcal{PT} symmetry, and in particular, the asymptotically non-vanishing potential component has strong influence on the asymptotic properties of the wave functions, and this fact manifests itself in the structure of the transmission and reflection coefficients too, in accordance with the findings of [22]. It turns out that for real E (as is the case here) the asymptotically vanishing (i.e. bound) states can be identified with the *zeros* of the reflection coefficients, rather than with the poles of the transmission (and reflection) coefficients. The reason is that in these solutions $\exp(\pm ip_{\pm} x)$ occur with the same sign in the exponent for both $x > 0$ and $x < 0$, corresponding to a transmitting wave. In particular, for the potential (33) the bound state occurs for $2p_{+I} + \gamma = 0$, which is the zero of (39), while for the reverse direction, the zero of $R_{R \rightarrow L}$ occurs at $2p_{-I} + \gamma = 0 = -2p_{+I} + \gamma$ corresponding to the interchange of p_- and p_+ or spatial reflection. The same results are obtained from the discussion of Section 2 too.

4. CONCLUSIONS

We investigated the \mathcal{PT} -symmetric Rosen–Morse II and finite square well potentials in the limit when their real even potential component turns into the Dirac delta, while their imaginary odd component tend to the sign function, respectively.

The energy spectrum was found to contain a single real eigenvalue for $\gamma < 0$ and arbitrary Λ , depending on both parameters. The transmission and reflection coefficients were also determined, and it was found that they exhibit the expected handedness effect. The results of [24] were recovered for the bound-state energy after setting $\Lambda = 1/2$, while for $\Lambda = 0$ the Dirac delta potential was obtained. The results were also derived for the hermitian version of this potential with an imaginary Λ .

The transmission and reflection coefficients were also considered in the appropriate limit for the two potentials. It was confirmed that the handedness effect occurs in this case too, i.e. in contrast with real potentials, the reflection coefficients differ essentially for waves arriving from the two directions, while the transmission coefficients differ only in a phase. (Note that for potentials with asymptotically vanishing imaginary component even this phase is missing.) It was shown that the only bound state that occurs in the limiting case from both potentials is obtained as the zero of the reflection coefficient, rather than as the pole of the transmission coefficient, in accordance with the findings of [22].

The present study confirms the importance of the asymptotically non-vanishing imaginary potential component, which was already pointed out in connection with the \mathcal{PT} -symmetric Rosen–Morse II potential [10, 21]. It is notable that supplementing the same real even asymptotically vanishing potential component with an asymptotically vanishing odd imaginary potential component (Scarf II [15, 29]) leads to complex conjugate energy eigenvalues when the relative intensity of the imaginary component is increased, but this phenomenon does not occur when the imaginary potential component is chosen asymptotically non-vanishing (Rosen–Morse II). In this case increasing the intensity of the imaginary component leads to lifting the energy spectrum to higher energies, such that even the ground-state energy can be tuned to positive values. This was also found for the \mathcal{PT} -symmetric finite square well [22] potential.

It is instructive to consider further \mathcal{PT} -symmetric potentials with various asymptotic behaviour. The energy spectrum of the Bender–Boettcher potentials $V(x) = x^2(ix)^\varepsilon$ [1] contains complex conjugate energy eigenvalues for $\varepsilon < 2$. In this case complexification is a gradual process, starting from higher energies. For $\varepsilon \geq 0$ the energy eigenvalues are all real, similarly to the case of the \mathcal{PT} -symmetric Rosen–Morse II potential. The $\varepsilon = 1$ choice recovers the purely imaginary ix^3 potential.

Another interesting case is the \mathcal{PT} -symmetric exponential potential [20]. Its solutions are expressed in terms of Bessel functions, so it is also outside the Natanzon class. This two-parameter potential is purely imaginary, and it tends to infinity asymptotically stronger than the imaginary component of the Bender–Boettcher potential. It has the unusual feature that its energy spectrum generally contains both real and complex energy eigenvalues such that it is not possible to separate parametric domains where only imaginary energy eigenvalues occur. Increasing non-hermiticity leads to the gradual complexification of the energy spectrum from above, however, the ground-state energy always remains real.

All these findings indicate that the breakdown of \mathcal{PT} symmetry occurs in potentials with rather different patterns of the imaginary component. For asymptotically strongly divergent imaginary potential components the complexification of the energy eigenvalues generally occurs gradually, starting from above. For potentials with asymptotically vanishing imaginary component the same procedure occurs from below either suddenly [15–17] or gradually [18], but in these cases a non-vanishing real potential component is also necessary to obtain bound states.

It is notable that although potentials with asymptotically constant imaginary potential component (such as the Rosen–Morse II and its limit discussed here) fall between the two potential types mentioned above, their energy spectrum is purely real. Furthermore, a real potential component is also necessary for them to support bound states. Further studies concerning potentials with various asymptotic patterns seem worthwhile in order to shed more light on the possible mechanisms of the breakdown of \mathcal{PT} symmetry.

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