\textbf{\Large $\mathcal{PT}$-symmetry breaking with divergent potentials: lattice and continuum cases}

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We investigate the parity- and time-reversal ($\mathcal{PT}$)-symmetry breaking in lattice models in the presence of long-ranged, non-hermitian, $\mathcal{PT}$-symmetric potentials that remain finite or become divergent in the continuum limit. By scaling analysis of the fragile $\mathcal{PT}$ threshold for an open finite lattice, we show that continuum loss-gain potentials $V_{\alpha}(x) \propto |x|^\alpha \text{sign}(x)$ have a positive $\mathcal{PT}$-breaking threshold for $\alpha > -2$, and a zero threshold for $\alpha \leq -2$. When $\alpha < 0$ localized states with complex (conjugate) energies in the continuum energy-band occur at higher loss-gain strengths. We investigate the signatures of $\mathcal{PT}$-symmetry breaking in coupled waveguides, and show that the emergence of localized states dramatically shortens the relevant time-scale in the $\mathcal{PT}$-symmetry broken region.

\section{INTRODUCTION}

Since Bender and co-workers' seminal work on non-hermitian Hamiltonians a decade and a half ago, there has been tremendous progress in the field of parity and time-reversal ($\mathcal{PT}$)- symmetric quantum theory [13]. For continuum, $\mathcal{PT}$-symmetric, non-hermitian Hamiltonians on an infinite line, they showed that the eigenvalue spectrum is purely real when the strength of the “non-hermiticity” is small, and becomes complex when it is large. Traditionally, the region of the parameter space where the eigenvalues of the $\mathcal{PT}$-symmetric Hamiltonian are purely real, $\epsilon_\lambda = \epsilon_\lambda^*$, and the non-orthogonal eigenfunctions are simultaneous eigenfunctions of the combined $\mathcal{PT}$-operation, $f_\lambda(x) = f_\lambda^*(-x)$, is called the $\mathcal{PT}$-symmetric region. In the early years, significant theoretical progress was made towards the development of a self-consistent quantum theory via a Hamiltonian-dependent inner product, under which the eigenfunctions become orthonormal in the $\mathcal{PT}$-symmetric phase [2]. This progress was accompanied by mathematical advances in the field of pseudohermitian operators - operators that are not hermitian under the standard inner product, but may be self-adjoint under an appropriately defined metric [3]. Most of these investigations were focused on continuum Hamiltonians on an infinite line.

During the past five years, discrete $\mathcal{PT}$-symmetric Hamiltonians on finite lattices and continuum $\mathcal{PT}$-symmetric Hamiltonians on a finite line have been extensively studied due to their experimental relevance. It has become clear that such Hamiltonians naturally arise as “effective Hamiltonians” for open systems with balanced loss and gain. Therefore $\mathcal{PT}$-symmetry breaking experimentally manifests in such systems as a transition from a quasiequilibrium state to a state with broken reciprocity. Experimental demonstrations of $\mathcal{PT}$-symmetry breaking in optics [5-8], and the natural emergence of $\mathcal{PT}$-symmetric effective potentials in driven condensed matter systems [11-19] have complemented theoretical studies of $\mathcal{PT}$-symmetry breaking in lattice models [14-19] and continuum models on a finite line [20-23]. Special attention has been paid to the number of eigenvalues that become complex [24], their location in the energy spectrum [25-26], the extended or localized nature of the corresponding eigenstates [27], and the experimental consequences of the spatial extent of the states that break the $\mathcal{PT}$ symmetry [28]. These developments suggest that understanding the differences [29] between finite and infinite lattice models is crucial for a detailed understanding of the $\mathcal{PT}$-symmetry breaking phenomenon, particularly because all of its realizations have been in small lattices with $N \lesssim 100$ sites.

Here, we investigate $\mathcal{PT}$-symmetry breaking in $N$-site lattices with extended loss-gain potentials characterized by strength $\gamma > 0$ and parameter $\alpha$, and their continuum counterparts on a finite line. The paper is organized as follows. In the next section, we present the tight-binding model, and discuss the $\mathcal{PT}$-symmetric threshold $\gamma_{\mathcal{PT}}(N, \alpha)$ results on the lattice and their continuum implications. In particular, we show that some divergent power-law potentials on a finite line have a positive $\mathcal{PT}$-symmetry breaking threshold. In Sec. III we discuss the signatures of $\mathcal{PT}$-symmetry breaking in such lattices, and show that they are consistent with the expectations based on the extended nature of $\mathcal{PT}$-broken eigenstates. In Sec. IV we show that localized states with complex energies in the band emerge at much larger loss-gain strength $\gamma_c \gg \gamma_{\mathcal{PT}}$, and discuss their significance. We conclude the paper with Sec. V.

\section{TIGHT-BINDING MODEL}

Consider an $N$-site tight-binding lattice with site-to-site distance $a$, nearest-neighbor tunneling $J > 0$, and open boundary conditions. Its hermitian tunneling Hamiltonian is given by

\begin{equation}
H_0 = -J \sum_{k=1}^{N-1} \left( a_{k+1}^\dagger a_k + a_k^\dagger a_{k+1} \right)
\end{equation}

where $a_k^\dagger (a_k)$ represents the creation (annihilation) operator for a state $|k\rangle$ localized at site $k$. We keep coupled optical waveguides in mind for an experimental realiza-
tion of this lattice; thus, $a^\dagger_1$ represents the creation operator for the single-mode electric field in the waveguide $1 \leq k \leq N$. The parity operator on an open lattice is given by $\mathcal{P} : a^\dagger_n \to a^\dagger_{N-n}$ where site $\bar{n} = N + 1 - n$ is the parity-symmetric counterpart of site $n$. The action of the time-reversal (or motion-reversal) operator is $\mathcal{T} : i \to -i$.

The spectrum of the tight-binding model is given by $E_n = -2J \cos(k_n)$, and the corresponding extended, normalized eigenfunctions are $\langle \bar{n} | \psi_n \rangle = \sin(k_n \bar{m})$. Here $k_n = n\pi/(N+1)$ with $1 \leq n \leq N$. Note that the spectrum is symmetric about zero, $E_n = -E_{\bar{n}}$, the eigenfunctions have equal weights on $\mathcal{PT}$-symmetric sites, and the eigenstates at energies $\pm E_n$ are related by $\langle m | \psi_n \rangle = (-1)^n \langle m | \psi_{\bar{n}} \rangle$. These symmetries of the spectrum and eigenfunctions remain valid in the presence of pure loss-gain potentials in the $\mathcal{PT}$-symmetric region [30].

We consider a class of extended loss-gain potentials parameterized by $\alpha$,

$$V_\alpha = i\gamma \sum_{k=1}^{N} (k - n_c)^\alpha \text{sign}(k - n_c) a^\dagger_k a_k. \quad (2)$$

Here, $\gamma > 0$ is the strength of the potential and $n_c = (N+1)/2$ is the lattice center. With the present convention, the first half of the lattice, $k \leq n_c$, is the “loss region” and the second half of the lattice, $k > n_c$, is the “gain region”. The continuum limit of this problem is defined by $N, J \to \infty$ and $a \to 0$ in such a manner that $Na \to 2L$ defines the size of the box and $Ja^2 \to \hbar^2/2m$ defines the mass of the non-relativistic quantum particle confined in this one-dimensional box. With this notation, it follows that the continuum potential becomes

$$V_\alpha(x) = i\Gamma|x/L|^\alpha \text{sign}(x) = V_\alpha^*(-x), \quad (3)$$

where the potential strength $\Gamma$ is given by

$$\Gamma = \lim_{N \to \infty} \gamma \left( \frac{N}{2} \right)^\alpha. \quad (4)$$

Thus, the continuum problem corresponding to the Hamiltonian $H_0 + V_\alpha$ is given by the Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V_\alpha(x) \psi(x) = E \psi(x) \quad (5)$$

subject to boundary conditions $\psi(x = \pm L) = 0$. At this point, we remind the reader that extended potentials on a lattice, Eq. (2), were investigated and deemed unstable due to the vanishing $\mathcal{PT}$-symmetric threshold that is obtained in the limit $N \gg 1$ [10, 20]. On the other hand, corresponding $\mathcal{PT}$-potentials on a finite line, Eq. (3), such as $V(x) = ix$ [12] or $V(x) = is\text{sign}(x)$ [20] were found to have a positive $\mathcal{PT}$-breaking threshold. In this section, we resolve this apparent discrepancy between the lattice and continuum results.

Since the spectrum of the $\mathcal{PT}$-symmetric Hamiltonian $H_\alpha = H_0 + V_\alpha$ cannot be obtained analytically, we numerically obtain the threshold $\gamma_{\mathcal{PT}}(N, \alpha)$ below which all eigenvalues of the Hamiltonian are purely real. The left-hand panel in Fig. 1 shows the dependence of the threshold on the lattice size. We see that $\gamma_{\mathcal{PT}}(N, \alpha)/J$ decreases in a power-law fashion as the lattice size $N$ increases, and that the power-law exponent is determined by $\alpha$. Although these results are for $N=100-1000$, they hold true for any $\alpha > -2$. When $\alpha \leq -2$, the lattice threshold $\gamma_{\mathcal{PT}}(\alpha)/J \geq 0$ is independent of the lattice size $N$. Thus, for $\alpha > -2$, the $\mathcal{PT}$-symmetric phase with extended $\mathcal{PT}$-potentials is fragile [31], but in a very specific
manner,
\[
\gamma_{PT}(N, \alpha) = A_\alpha \left( \frac{2}{N} \right)^{\alpha+2}.
\]
(6)

It follows from Eqs. (4) and (6) that the dimensionless continuum threshold for \(V_\alpha(x)\) is equal to the power-law prefactor,
\[
\Gamma_{PT}(\alpha) = \lim_{N \to \infty} \gamma_{PT} \left( \frac{N}{2} \right)^{\alpha+2} = A_\alpha,
\]
(7)
where \(E_L = \hbar^2/2mL^2\). Thus, the fragile nature of the \(PT\)-symmetric phase on the lattice scale for \(\alpha > -2\) implies a positive threshold for the counterpart potential for a particle in a box on the continuum scale. This continuum threshold \(\Gamma_{PT}\) obtained from the scaling data is shown in the right-hand panel of Fig. 1. It shows that \(\Gamma_{PT}(\alpha)/E_L\) is a positive, monotonically increasing function of \(\alpha\) that goes to zero as \(\alpha \to -2^+\). The threshold \(\Gamma_{PT}(\alpha)/E_L = 0\) for \(\alpha \leq -2\) since the corresponding lattice threshold is independent of \(N\). These results imply that, surprisingly, divergent \(PT\) potentials including \(V(x) = \Delta(L/x)\) have a nonzero \(PT\)-breaking threshold.

We emphasize here that a similar problem on the infinite line, studied by Bender et al. [1] leads to very different results. In their spectrum, the curve is purely real when \(\alpha \geq 2\) and has no real eigenvalues for \(\alpha \leq 1\) irrespective of the strength \(\Gamma\) of the potential. In our case, the compact nature of the support of all eigenfunctions leads to a characteristic energy-scale \(E_L\), and therefore we obtain a finite \(PT\)-breaking threshold that is determined by the potential-strength \(\Gamma/E_L\). We also note that the \(PT\)-symmetry breaking on a finite line occurs when the lowest two energy levels, the ground state and the first excited state, become degenerate and then complex [12, 20, 32]. In contrast, \(PT\)-symmetry breaking occurs in (highly) excited states for the corresponding problem on an infinite line [13]. These salient differences show that \(PT\) symmetry breaking on a finite line, best modeled via a discretized lattice, is qualitatively different from \(PT\)-symmetry breaking in continuum potentials on an infinite line [33]. In the following section, we investigate the signatures of such \(PT\) symmetry breaking.

III. \(PT\) BREAKING SIGNATURES

The lattice Hamiltonian \(H_\alpha\) can be realized in an array of coupled optical waveguides. The tunneling \(J\) is determined by the waveguide cross-section and the distance between adjacent waveguides. It is easily tuned with present-day technology [34–36], as is the loss potential in the first half of the lattice, \(k \leq n_e\), engineered via the imaginary part of the index of refraction. The fabrication of an extended, position-dependent gain potential has not yet been experimentally demonstrated, although it is relatively straightforward to implement in the discrete parity-time synthetic lattices [37, 38]. In this section, we present the signatures of \(PT\)-symmetry breaking in the time-evolution of an initially normalized wave packet, and discuss their relationship with the spatial structure of \(PT\)-broken eigenfunctions.

Since \(H_\alpha\) is a single-particle, time-independent Hamiltonian, it is straightforward to obtain the time-evolved state \(|\psi(t)\rangle = G(t)|\psi(0)\rangle\) where \(G(t) = \exp(-iH_\alpha t/\hbar)\) is the non-unitary time evolution operator. The site-and time-dependent intensity is then obtained as \(I(k, t) = |\langle k|\psi(t)\rangle|^2\), and the total intensity \(I(t) = \sum_k I(k, t)\) is not conserved. Note that since the finite-dimensional Hamiltonian \(H_\alpha\) is diagonalizable, the net intensity \(I(t)\) oscillates but remains bounded when \(\gamma < \gamma_{PT}\) and increases exponentially with time at long times when \(\gamma > \gamma_{PT}\).

At the \(PT\)-breaking point, the Hamiltonian is defective, and can be reduced to a Jordan canonical form. Therefore, at long times, the net intensity scales as a power-law, \(I(t) \propto t^{2(p-1)}\), where \(p \geq 2\) is the dimension of the Jordan block corresponding to the \(PT\)-breaking, degenerate eigenvalue. Thus, for any finite lattice, at the \(PT\)-breaking threshold, the net intensity at long times scales as an even power of time or, equivalently, the distance along the waveguide. We will see in the next section that the relevant time-scale that codifies “long time” is crucially determined by the extended vs. localized nature of eigenfunctions with complex energies.

We use an initial state centered at \(k_0\),

\[
\langle k|\psi(0)\rangle = \frac{1}{A} e^{-(k-k_0)^2/2\sigma^2}
\]

(8)
where \(A^2(\sigma, N, k_0) = \sum_{k=1}^N \exp\left[-(k-k_0)^2/\sigma^2\right]\) ensures that the state is normalized. The results shown in Fig. 2 are for \(\sigma = 1\) and \(k_0 = n_e\) - the state is essentially localized on sites \(N/2\) and \(N/2 + 1\) - and one obtains qualitatively similar results for broad wave packets centered at arbitrary locations. The left-hand column in Fig. 2 shows \(I(k, t)\) for \(\alpha = +1\) (top panel), \(\alpha = 0\) (center panel), and \(\alpha = -1\) (bottom panel). In each case, the \(PT\)-potential strength is just below the threshold, \(\gamma/\gamma_{PT}(N, \alpha) = 0.995\), the unit of time is given by \(T_s = 2\pi/\Delta_v\) where the average level spacing is \(\Delta_v \sim 4J/N\) (\(\hbar = 1\)). We have chosen the time-range \(t/T_s \leq 150\) to cover one bounded intensity oscillation. The top panel shows that when \(\alpha = +1\), the wave packet undergoes amplification near the center of the lattice. The region of maximal intensity is spread out broadly at \(\alpha = 0\) (center panel), whereas when \(\alpha = -1\), the maximum amplification does not occur near the center of the lattice. In each case maximum site-intensity in the loss region, \(k \leq n_e\), lags the maximum site-intensity in the gain region, \(k > n_e\). The right-hand column shows that just above the threshold, \(\gamma/\gamma_{PT}(N, \alpha) = 1.005\), the intensity profile monotonically increases with time, but retains an identical \(\alpha\)-dependence.

These intensity profiles, before the \(PT\)-breaking and after, have two surprising features. The first is that the
amplification in the gain region is faithfully transferred to the loss region. Thus, the lag between the intensity maxima is the primary distinguisher between gain and loss regions. The second is that the maximum site intensity does not occur in the region of maximum gain potential. When \( \gamma > 0 \), the loss-gain maxima occur at the edges of the lattice and the intensity maxima from the non-unitary time evolution are concentrated near the center. When \( \gamma < 0 \), the loss-gain maxima occur at the center of the lattice, whereas the intensity maxima are displaced outward. This counterintuitive behavior is understood by focusing on the eigenfunctions that break the \( \mathcal{PT} \)-symmetry and dominate the non-unitary time evolution. At \( \gamma = 0 \), the ground state wave function \( \psi_1(k) = \sin(\pi k/(N + 1)) \), and the excited state wave function \( \psi_2(k) = \sin(2\pi k/(N + 1)) \) are orthogonal. As \( \gamma \to \gamma_{PT} \), the corresponding \( \gamma \)-dependent eigenfunctions become degenerate, and show a maximum at the center of the lattice for \( \gamma > 0 \) and a dip at the center of the lattice for \( \gamma < 0 \). Indeed, at long times, the intensity profile \( I(k,t) \) is determined by the intensity profile of these eigenfunctions and is therefore (mostly) independent of the choice of the initial state \( |\psi(0)\rangle \).

For all potentials \( V_\alpha \) considered in this paper, the \( \mathcal{PT} \)-symmetry is first broken via the ground-state and first-excited-state eigenfunctions that are extended over the entire lattice. When the potential strength exceeds the fragile threshold \( \gamma_{PT}(N,\alpha) \propto J(2/N)^{\alpha+2} \) and continues to increase, the fraction of eigenvalues that become degenerate and then complex increases, and the corresponding extended eigenfunctions become \( \mathcal{PT} \)-asymmetric. In the following section, we will investigate the emergence of localized states with complex energies in the \( \mathcal{PT} \)-broken spectrum that occurs at \( \gamma \sim J \gg \gamma_{PT}(N,\alpha) \).

**IV. BOUND STATES IN THE CONTINUUM**

The discrete spectrum of the Hamiltonian \( H_0 \) is bounded by \( \pm 2J \) and becomes a continuous band when the lattice is infinite. A remarkable property of the Hamiltonian \( H_\alpha \) is that, no matter how “strong” the loss-gain potential is, the real part of the energy spectrum of \( H_\alpha \) remains confined to this band while the imaginary part of complex energies increases with the loss-gain strength for \( \gamma \gg \gamma_{PT} \). Just as bound states occur in the presence of a hermitian potential, they do in the presence of a non-hermitian, \( \mathcal{PT} \)-symmetric potential when its strength exceeds a threshold \( \gamma_c \). The crucial difference in the latter case, though, is that the (real part of) energy of such localized states lies in the band \( \pm 2J \). It is possible to analytically obtain the threshold \( \gamma_c \) for a single pair of \( \mathcal{PT} \) impurities in an infinite lattice [27, 29]. However, in the present case with extended potentials \( V_\alpha \), we locate this threshold numerically.

Figure 3 shows the bound-state threshold \( \gamma_c(\alpha)/J \) for an infinite lattice, obtained from the data for lattice sizes \( N=100-4000 \). When \( \alpha > 0 \), the potential does not have any bound states. As \( \alpha \) decreases, the potential deepens near the center and bound states localized near the lattice-center emerge. We find that the requisite threshold \( \gamma_c(\alpha)/J \) decreases monotonically with de-
increasing $\alpha \leq -1$. This is consistent with the fact that for large, negative $\alpha$, the potential is increasingly concentrated near the lattice center, and therefore the threshold strength necessary to support a bound state is lowered. When $-1 < \alpha < 0$, the cumulative potential strength,

$$V_c(\alpha) = \sum_{k > n_c}^N \frac{1}{(k - n_c)^\alpha}$$

diverges as $N \to \infty$. Therefore the threshold strength $\gamma_c(\alpha)$ required for a bound state vanishes in this limit. We emphasize that the bound-state threshold value is much larger than the $PT$-symmetry breaking threshold for the same lattice, $\gamma_c(\alpha)/J \sim 1 \gg \gamma_{PT}(\alpha, N)/J$.

The inset in Fig. 3 shows the emergence of a bound state at $\alpha = -1$, which implies $\gamma_c/J = 1$. The horizontal axis represents fractional location along the lattice, and the vertical axis denotes site intensity; the solid lines represent results for $N = 200$ and the dashed lines correspond to the $N = 400$ case. When $\gamma/\gamma_c = 0.95$, the eigenstate site-intensity is nonzero over the entire gain region. (The eigenstate with the complex-conjugate energy has site-intensity that is nonzero over the entire loss region.) As is expected for an extended state, when the lattice size is doubled from $N = 200$ (red solid line) to $N = 400$ (red dashed line) the site-intensity height is reduced by a factor of two. This changes dramatically as $\gamma$ crosses the bound-state threshold. At $\gamma_c/J = 1.05$, the corresponding eigenstate now becomes localized near the lattice center in the gain region. We note that in contrast to the extended state, the localized state site-intensity profiles for $N = 200$ (blue solid line) and $N = 400$ (blue dashed line) have the same height, and the fractional width of the profile is halved as $N$ is doubled. This is the key signature of a localized state.

Lastly, we demonstrate the dramatic effect of the emergence of a localized state with complex energy on the time-scale that determines the “long-time” behavior of net intensity $I(t)$ in the $PT$-symmetry broken phase, and present the behavior of the intensity at much shorter time-scales. All results in Fig. 4 are obtained for an $N = 100$ lattice with $\alpha = -1$, and an initial state at the center of the lattice, $Eq. (8)$, with $\sigma = 10$. Panel (a) in Fig. 4 shows that the net intensity $I(t)$ increases exponentially at times $tE_L \gg 20$ where $1/E_L$ represents the time-scale associated with extended states that break the $PT$ symmetry. Recall that this time-scale is much longer than the bound-state time-scale, $1/E_L = (1/J)(N/2)^2 \gg 1/J$. Panel (b) in Fig. 4 shows the behavior of net intensity $I(t)$ over time-scale $1/J$. Below the bound-state threshold, $\gamma_c/J = 0.998$ (blue solid line), the intensity on the logarithmic scale shows a step-like structure. This step-structure is replaced by a straight line just above the threshold, $\gamma_c/J = 1.006$ (red dot-dashed line). Thus, the presence of a localized state with complex energy dramatically shortens the time-scale for exponential intensity behavior from $\sim 1/E_L$ to $\sim 1/J \ll 1/E_L$. Panel (c) in
Fig. 4 shows the logarithm of site and time-dependent intensity $I(k, t)$ just below the bound-state threshold, $\gamma/\gamma_c = 0.998$. The vertical white dashed line marks the time when the first partial waves, starting near the center of the lattice, return to the center after reflection at the two ends of the open lattice; these return reflections are denoted by white dotted lines. Panel (c) $I(k, t)$ and panel (b) $I(t)$ show that the step-structure in the intensity, denoted by a vertical dotted black line, corresponds to the return of such partial waves. Below the bound-state threshold, such staircase structure in the net intensity $I(t)$ is exhibited at times $T_n = nN/2J$.

V. DISCUSSION

In this paper, we have investigated $\mathcal{PT}$-symmetry breaking in the presence of extended potentials on a lattice, some of whom map onto divergent potentials on a finite line in the continuum limit. We have shown that the algebraically fragile $\mathcal{PT}$-breaking threshold in lattice models with extended loss-gain potentials guarantees a positive, finite threshold in its continuum counterparts.

In addition, we have found that divergent, loss-gain potentials such as $V(x) \propto i/x$ on a finite line have a positive $\mathcal{PT}$-breaking threshold. We have shown that the emergence of localized states in $\mathcal{PT}$ potentials dramatically shortens the time-scale required necessary for the net intensity to exhibit exponential behavior.

Our results elucidate the connection between finite lattice models and their continuum limit, and raise similar questions about $\mathcal{PT}$-symmetry breaking in exactly infinite lattices and their counterparts on an infinite line. They hint at the existence of analytical solutions for special values of $\alpha$, such as $\alpha = -2$ or $\alpha = -1$. Addressing these questions will deepen our understanding of $\mathcal{PT}$-symmetry breaking and its observable consequences in experimentally accessible finite lattice systems.

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