The robust $\mathcal{PT}$-symmetric chain and properties of its Hermitian counterpart

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Abstract

We study the properties of a parity- and time-reversal- ($\mathcal{PT}$) symmetric tight-binding chain of size $N$ with position-dependent hopping amplitude. In contrast to the fragile $\mathcal{PT}$-symmetric phase of a chain with constant hopping and imaginary impurity potentials, we show that, under very general conditions, our model is always in the $\mathcal{PT}$-symmetric phase. We numerically obtain the energy spectrum and the density of states of such a chain, and show that they are widely tunable. By studying the size-dependence of inverse participation ratios, we show that although the chain is not translationally invariant, most of its eigenstates are extended. Our results indicate that tight-binding models with non-Hermitian, $\mathcal{PT}$-symmetric hopping have a robust $\mathcal{PT}$-symmetric phase and rich dynamics which may be explored in coupled waveguides.
Introduction: Since the seminal paper by Bender et al. [1] a decade ago, it has become clear that non-Hermitian Hamiltonians with parity and time-reversal ($\mathcal{PT}$)-symmetry can have purely real spectra [2, 3] and, with an appropriately redefined inner-product, they lead to orthogonal eigenvectors [2], unitary scattering [4] and, therefore, a consistent quantum theory. The theoretical work on continuum, $\mathcal{PT}$-symmetric, non-Hermitian Hamiltonians [5] since then has been accompanied, most recently, by experiments in optics where spontaneous $\mathcal{PT}$-symmetry breaking in a classical system has been observed in waveguides with $\mathcal{PT}$-symmetric complex refractive index [6, 7] and by theoretical studies of distributed-feedback optical structures that can be mapped onto a relativistic, $\mathcal{PT}$-symmetric Hamiltonian [8].

Idealized lattice models have been popular in physics due to their analytical and numerical tractability, the absence of divergences [9], the availability of exact solutions [10], and the ability to capture counter-intuitive physical phenomena [11]. As with the standard quantum theory, these models have been based on Hermitian Hamiltonians. In recent years, tight-binding models with a Hermitian hopping and $\mathcal{PT}$-symmetric, complex, on-site potentials [12–14], non-Hermitian transitions [15], and $\mathcal{PT}$-symmetric spin-chains [16] have been extensively explored. For a tight-binding chain with $\mathcal{PT}$-symmetric impurity potentials, a salient result is that its $\mathcal{PT}$-symmetric phase - the range of model parameters that lead to a real spectrum - is extremely fragile [12, 14]. This fragile nature of the $\mathcal{PT}$-symmetric phase precludes effects such as the Anderson localization [17], impurity-bound states [18], and the Luttinger-liquid behavior [19] in such a chain with a non-Hermitian Hamiltonian.

In this paper, we explore the properties of a tight-binding chain of size $N$ with $\mathcal{PT}$-symmetric, non-Hermitian, position-dependent hopping amplitudes. Our main results are as follows: (i) We show that the system is always in the $\mathcal{PT}$-symmetric phase under very general criteria that we derive. (ii) The energy spectrum and the resulting density of states in such a chain are widely tunable and symmetric around zero. (iii) Although the chain is not translationally invariant, (a majority of) its eigenfunctions are delocalized. Our results show that a robust $\mathcal{PT}$-symmetric chain has non-Hermitian hopping amplitudes and Hermitian potentials, and that its Hamiltonian is similar to that of a chain with position-dependent, parity-symmetric hopping [20].

Tight-binding Model: We start with a Hamiltonian for an $N$-site tight-binding chain,

$$H_{\mathcal{PT}} = - \sum_{i=1}^{N-1} \left( t_{i} c_{i+1}^\dagger c_{i} + t_{N-i}^* c_{i}^\dagger c_{i+1} \right)$$

(1)
where $c_n^\dagger(c_n)$ is the creation (annihilation) operator at site $n$, $t_i$ are the position-dependent hopping amplitudes, and the asterisk denotes complex conjugation. The parity operator on the chain is given by $\langle m|P|n \rangle = \delta_{m,N+1-n} = \delta_{m,\bar{n}}$ where $|m\rangle$ represents a single-particle state localized at site $m$, and $\bar{m} = N + 1 - m$ is the reflection-counterpart of site $m$; it follows that $H_{PT}$, although not Hermitian, is $\mathcal{PT}$-symmetric. We consider only the single-particle sector and, since periodic boundary conditions are incompatible with the $\mathcal{PT}$-symmetry, use open boundary conditions. Numerical results indicate that the spectrum of $H_{PT}$ is purely real when the hopping elements have the same sign; in the following paragraph, we analytically derive the criteria that guarantee this robustness.

Let us consider a similarity transformation \[5\] of the non-Hermitian Hamiltonian, $H_{PT} \rightarrow H = M^{-1}H_{PT}M$ where $M = \text{diag}(m_1, \ldots, m_N)$ is a diagonal matrix. It is straightforward to show that the transformed matrix $H$ is Hermitian, $H = H^\dagger$, if and only if

$$\frac{m_{k+1}^* m_{k+1}^*}{m_k^* m_k} = \left(\frac{t_{N-k}}{t_k}\right) > 0.\quad (2)$$

We note that this constraint only applies to a diagonal $M$. Thus, the $\mathcal{PT}$-symmetric Hamiltonian $H_{PT}$ is similar to a Hermitian Hamiltonian $H$ if and only if the phases of the hopping amplitudes $(t_k, t_{N-k})$ are the same for all $k = \{1, \ldots, N - 1\}$. When the hopping elements are real, it implies that $t_k$ and $t_{N-k}$ must have the same sign; when they are complex, $t_m = |t_m| \exp(i\theta_m)$, it implies that $\theta_k = \theta_{N-k}$. The eigenvalue spectrum of the non-Hermitian Hamiltonian $H_{PT}$ is purely real, as long as these general requirements are satisfied. Since $H = M^{-1}H_{PT}M = H^\dagger$, it follows that the eigenvalues $E_n$ of $H$ and $H_{PT}$ are the same, and that the orthogonal eigenvectors of $H$, $H|v_n\rangle = E_n|v_n\rangle$, and the (non-orthogonal) eigenvectors of the $\mathcal{PT}$-symmetric Hamiltonian, $H_{PT}|u_n\rangle = E_n|u_n\rangle$ are related by $|u_n\rangle = M|v_n\rangle$. This relation provides the requisite inner-product under which the eigenvectors $|u_n\rangle$ of $H_{PT}$ are orthonormalized. We note this transformation corresponds to the positive-definite, self-adjoint, invertible metric $\eta^{-1} = MM^\dagger$. \[16\]

The hopping amplitudes for atomic orbitals can be, in general, complex \[21\]. However, for optical lattices, coupled waveguides, or superlattices, the hopping amplitude, determined by the overlap of adjacent on-site (Gaussian or exponential) ground-state wavefunctions, is positive, just as it is for $s$-wave atomic orbitals \[21\]. A truly non-Hermitian Hamiltonian $H_{PT}$ may be realized in systems with asymmetrical hopping due to an in-plane field \[22\] or a voltage bias \[23\]. Its Hermitian counterpart $H$, with position-dependent, parity symmetric
hopping, may be realized in evanescently coupled waveguides where the wavepacket evolution and two-particle quantum correlations are exquisitely sensitive to the hopping \[20\].

Note that Eq.(2), although dependent upon the underlying Hamiltonian $H_{PT}$, does not uniquely determine the transformation matrix $M$ or the Hermitian matrix $H$. For simplicity, we choose $M$ to be real and $m_1 = 1$ which implies, via $m_{k+1} = m_k \sqrt{t_{N-k}/t_k}$, that $m_N = 1$. The resulting real matrix $M$ commutes individually with the parity- and time-reversal operators. Since numerical diagonalization of a Hermitian matrix $H$ is faster and more accurate than its non-Hermitian counterpart $H_{PT}$, in numerical calculations we use its Hermitian counterpart $H$ with entries

$$H_{mn} = -|t_{m}t_{N-m}|^{1/2} \left( \delta_{m,n-1}e^{i\theta_m} + \delta_{m-1,n}e^{-i\theta_{N-n}} \right),$$

where we recall that $\theta_{N-n} = \theta_n$. In the following sections, we discuss basic properties of such a chain, with focus on the energy spectrum and nature of wavefunctions of $H$ when the hopping is not uniform.

**Energy Spectrum and Density of States:** We start with numerical results for an $N = 500$ site chain with hopping amplitude given by $t_k = t_0k^\alpha$ where $t_0$ sets the hopping-energy scale. When $\alpha = 0$, we have a uniform tight-binding chain, the energy spectrum is given by $E_n = -2t_0 \cos(k_n)$ where $k_n = n\pi/(N+1)$ for an open chain, and the density of states $\rho_0(x) = \theta(1-|x|)/2\pi t_0 \sqrt{1-x^2}$ diverges near the band edges $x = \pm 1$, where $x = E/(2t_0)$ and $\theta(x)$ is the Heaviside function. The left panel in Fig. 1 shows the cosine-spectrum for $\alpha = 0$ (black solid line), a linear spectrum that is obtained when $\alpha = 1$ (green dotted line), and nonlinear spectra obtained when $\alpha = 2$ (red dashed line) and $\alpha = -1$ (blue dot-dashed line). As is expected for a tight-binding model, the energy spectra are symmetric around zero $[24]$. These results show that the energy spectrum of the $\mathcal{PT}$-symmetric chain can be widely tuned. We note that when $\alpha < 0$, the eigenstates near the top and the bottom of the energy band are localized at the two ends of the chain.

The right panel in Fig. 1 shows the corresponding (un-normalized) densities of states $\rho_\alpha(E)$. It is clear that the density of states changes dramatically from $\rho_0(E)$ (black solid line) when $\alpha \neq 0$. When $\alpha = 1$, due to the linear spectrum, the density of states is constant. It develops a single peak at $E = 0$ and tapers off to a finite value at the band edges when $\alpha > 1$. In contrast, when $\alpha < 0$, it develops two symmetrical peaks and vanishes at the band edges for $N \to \infty$. We emphasize that when $\alpha \neq 0$, the system is not translationally
FIG. 1. (color online) (a) Left panel shows energy spectra for the robust $\mathcal{PT}$-symmetric chain, Eq. (1), with $N = 500$ sites and a position-dependent hopping amplitude $t_k = t_0 k^\alpha$ with $\alpha = \{0, 1, 2, -1\}$. The energy is normalized by its maximum value. When $\alpha = 0$ (black solid line), we recover the well-known tight-binding chain dispersion $E_n/(2t_0) = -\cos(k_n)$. When $\alpha = 1$ (green dotted line), we get a linear spectrum. When $\alpha > 1$ (red dashed line), the energy spectrum develops an inflection point at zero energy. In contrast, when $\alpha = -1$ (blue dot-dashed line), the energy spectrum is linear at the origin, has a steep slope near the band extrema, and develops two symmetrical inflection points. (b) Right panel shows corresponding (un-normalized) densities of states $\rho_\alpha(E)$. When $\alpha = 2 > 1$ (red dashed line), $\rho_{\alpha=2}(E)$ develops a maximum at zero energy and it monotonically decreases to a finite value at the band edges. When $\alpha = -1 < 0$ (blue dot-dashed line), the density of states shows a two-peak structure. When $\alpha = 0$ (black solid line), we recover the well-known result $\rho_0(E)$ that diverges at the band edges. These results show that the energy spectrum and density of states are widely tunable through the exponent $\alpha$.

invariant and therefore the quantum number $n$ is not associated with the momentum.

We now focus on $\alpha = 1$ or equivalently $t_k = t_0 k$ for $k = \{1, \ldots, N-1\}$. The band-edges in this case are given by $\pm E_0 = \pm (N-1)t_0$ and the uniform level-spacing is $\Delta E = E_{n+1} - E_n = 2t_0$. It follows from Eq. (1) that the recurrence relation satisfied by the coefficients of an
eigenfunction $|\psi_\gamma\rangle = \sum_{k=1}^{N} f^\gamma_k |k\rangle$ of $H_{PT}$ is

$$-t_0 \left[ k f^\gamma_{k+1} + (N + 1 - k) f^\gamma_{k-1} \right] = E^\gamma f^\gamma_k. \quad (4)$$

It is easy to check that $f^G_k = C^{N-1}_{N-k} = (N-1)!/(k-1)!(N-k)!$ satisfies Eq. (4) with eigenvalue $E^G = -(N-1)t_0$. Thus the ground-state wavefunction is $|\psi_G\rangle = \sum_{i=1}^{N} f^G_i |i\rangle$. Note that for $k \sim N/2 \gg 1$, Stirling approximation implies that the ground-state wavefunction is Gaussian near the center of the chain, $f^G_k \sim \exp\left[-(k-N/2)^2/2N^2\right]$. The first excited-state wavefunction is given by $f^1_k = (N + 1 - 2k)f^G_k$. It has energy $-(N-3)t_0$, and Stirling approximation shows that in the large $N$-limit, it carries over to the wavefunction for the first excited state of a simple harmonic oscillator. It is straightforward, but tedious, to construct the higher excited states. We emphasize that for every eigenstate with energy $-E < 0$, the eigenstate with energy $+E > 0$ is given by its staggered version: $f_k \rightarrow (-1)^k f_k$ [24].

When $\alpha \neq \{0, 1\}$ an analytical solution for the eigenvalue spectrum $H_{PT}$, or equivalently $H$, is unknown. However, the results in Fig. [1] for $\alpha > 0$ can be qualitatively understood with the simplest example of a non-trivial, symmetric, tridiagonal matrix $H$ with real entries $\{a, b, b, a\}$ above the diagonal. The matrix $H$ is similar to a $\mathcal{PT}$-symmetric Hamiltonian $H_{PT}$ of a 5-site chain with hopping parameters $\{t_1, t_2, t_3, t_4\}$ with $a = -\sqrt{t_1t_4}$ and $b = -\sqrt{t_2t_3}$. The eigenvalues of such a matrix are given by $E_n = \{\pm \sqrt{a^2 + 2b^2}, \pm a, 0\}$. For a position dependent hopping $t_k = t_0 k^\alpha$, when $\alpha = 0$ the slope of the energy spectrum at the band-edge is smaller than that at the origin, when $\alpha = 1$ we get the linear spectrum, and for $\alpha > 1$, the slope of the spectrum at the band-edge is larger than that at the origin.

Localized and Extended Wavefunctions: The $\mathcal{PT}$-symmetric chain with a position-dependent hopping is not translationally invariant, and when $\alpha \neq \{0,1\}$ its eigenfunctions are not analytically known. To study the evolution of the spatial extent of a wavefunction $|\psi\rangle = \sum_{i=1}^{N} f_i |i\rangle$ with increasing system size $N$, we calculate the inverse participation ratio (IPR) [25]

$$\text{IPR}_\psi(N) = \frac{\sum_{i=1}^{N} |f_i|^4}{\left( \sum_{i=1}^{N} |f_i|^2 \right)^2}. \quad (5)$$

If the IPR remains finite as $N \rightarrow \infty$, the wavefunction is localized whereas for an extended state, $\text{IPR}(N) \propto 1/N^\eta \rightarrow 0$ where $\eta > 0$; for a uniform tight-binding chain, $\alpha = 0$, the IPR$(N) = 3/N$ for all eigenstates. Note that the IPRs for eigenstates with energies $\pm E$ are the same. The left-panel in Fig. [2] shows the evolution of the maximum and minimum
FIG. 2. (color online) (a) The left-panel shows the minimum and maximum values of inverse-participation-ratio (IPR) for an $N$-site chain with Hamiltonian $H$, Eq. (3), as a function of position-dependent hopping $t_k = t_0 k^\alpha$. When $\alpha = 0$ (black solid circles), we obtain the analytical result $\text{IPR}(N) \propto 1/N$. The $\alpha = 1$ (blue dot-dashed line) and $\alpha = 2$ (red dashed line) results show that the IPRs decrease monotonically with increasing chain size. These results strongly suggest that all eigenstates are extended when $\alpha \geq 0$. (b) The right-panel shows the IPR results for $\alpha \leq 0$. The $\alpha = -1/2$ (blue solid circles) and $\alpha = -1$ (red open squares) results show that the minimum IPR is essentially independent of $\alpha$. The maximum IPR saturates to a nonzero value and indicates the presence of localized eigenstates with energies $\pm E$. These results show that when $\alpha < 0$, the system has both extended and localized states.

values of IPR for a chain with $N = 10$-5000 as a function of $\alpha \geq 0$. Note that since the chain size and the IPRs span decades, we use the logarithmic scale in Fig. 2. When $\alpha = 0$ (black solid circles) we obtain the analytical result, $\text{IPR}(N) = 3/N$. When $\alpha > 0$, we see that both the minimum and maximum IPRs decay with increasing chain size, max IPR $\propto N^{-\eta_\alpha}$ and min IPR $\propto N^{-\gamma_\alpha}$ where $0 < \eta_\alpha < \gamma_\alpha < 1$, and both exponents $\eta_\alpha$ and $\gamma_\alpha$ are monotonically decreasing functions of $\alpha$. These results strongly suggest that all eigenstates of the Hamiltonian $H$ with position-dependent hopping $t'_k = t_0 [k(N - k)]^{\alpha}/2$ are extended
when $\alpha \geq 0$. The right panel shows corresponding results for $\alpha \leq 0$. The minimum IPR is essentially independent of $\alpha$. On the other hand, in a sharp contrast with the previous results, we see that the maximum IPR quickly saturates to a nonzero value and indicates a localized state. Thus, when $\alpha < 0$, the system has both extended and localized eigenfunctions.

We note that these exponentially localized states, at the two ends of the chain, are essentially degenerate in energy; so are their staggered counterparts [24]. Thus, there are at least four eigenstates that have the same nonzero IPR. The qualitative difference between $\alpha > 0$ and $\alpha < 0$ cases can be attributed to the hopping: when $\alpha > 0$, the hopping amplitude increases from $\sim t_0 N^{\alpha/2}$ at the two edges to $\sim t_0 N^\alpha$ at the center of the chain, whereas when $\alpha < 0$, the hopping amplitude decreases from $\sim t_0/N^{\lvert \alpha \rvert/2}$ at the edges to $\sim t_0/N^{\lvert \alpha \rvert}$ at its center.

A better insight into the number of localized states is provided by the dependence of the IPR distribution on the size $N$ of the chain. Figure 3 shows the histogram of IPRs for $\alpha = 1$ (left column) and $\alpha = -1$ (right column). When $\alpha = 1$, as $N$ is increased tenfold from $N = 500$ (bottom-left panel) to $N = 5000$ (top-left panel), the entire IPR distribution shifts to smaller values. In contrast, when $\alpha = -1$, even as $N$ is increased tenfold, the IPR values for a few (localized edge) states, indicated by the red oval, are unchanged while the IPRs for the rest shift to lower values.

Discussion: $\mathcal{PT}$-symmetric lattices with a uniform hopping and imaginary impurities have an extremely fragile $\mathcal{PT}$-symmetric phase [12, 14]. In this paper, we have presented a tight-binding model with non-Hermitian, $\mathcal{PT}$-symmetric hopping, Eq.(1). We have shown that, under very general circumstances, this model is always in the $\mathcal{PT}$-symmetric phase, and its Hamiltonian is similar to a Hermitian Hamiltonian with position-dependent nearest-neighbor hopping, Eq.(3) [20]. These results are unaffected by the presence of ubiquitous, on-site, Hermitian disorder since it does not induce $\mathcal{PT}$-symmetry breaking.

Given the robust nature of the $\mathcal{PT}$-symmetric phase in this chain, we have explored its energy spectrum, density of states, nature of eigenfunctions, and their dependence on the functional form of the hopping amplitude $t_k = t_0 k^{\alpha}$. We find that when $\alpha = 1$ the energy spectrum is linear and gives rise to a constant density of states. We show that the energy spectrum is widely tunable by changing $\alpha$. We find that when $\alpha < 0$ the system has both localized and extended eigenfunctions in the absence of disorder, whereas when $\alpha > 0$, all eigenfunctions are extended. The effect of a Hermitian on-site disorder, then, is identical to that in a regular tight-binding model [17, 25]. Thus, the physics of the robust $\mathcal{PT}$-symmetric
FIG. 3. (color online) The evolution of the inverse-participation-ratio (IPR) distribution with the chain size $N$. Note the logarithmic scale. The top left and bottom left panels show that when $\alpha = 1$, as $N$ increases, the entire distribution of IPRs shifts to lower values. It suggests that all eigenstates of the Hamiltonian $H$, Eq.(3), are extended in the absence of disorder. The top right and bottom right panels show that when $\alpha = -1$, as $N$ is increased, although most of the IPRs shift to lower values, they saturate to a nonzero value for the states shown in the red oval. These eigenstates are localized at the two ends of the chain, and each finite value of the IPR is four-fold degenerate. Thus, when $\alpha < 0$, the system has both extended and localized eigenstates in the absence of disorder.

A chain with non-Hermitian hopping is extremely rich.

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