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

Yogesh N. Joglekar
Department of Physics, Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, Indiana 46202, USA

Avadh Saxena
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

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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.

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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] and, with an appropriately redefined inner product, they lead to orthogonal eigenvectors [2], unitary scattering [3], and, therefore, a consistent quantum theory. The theoretical work on continuum, $\mathcal{PT}$-symmetric, non-Hermitian Hamiltonians [4] 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 a $\mathcal{PT}$-symmetric complex refractive index [5,6] and by theoretical studies of distributed-feedback optical structures that can be mapped onto a relativistic, $\mathcal{PT}$-symmetric Hamiltonian [7].

Idealized lattice models have been popular in physics due to their analytical and numerical tractability, the absence of divergences [8], the availability of exact solutions [9], and the ability to capture counterintuitive physical phenomena [10]. 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 [11], non-Hermitian transitions [12], and $\mathcal{PT}$-symmetric spin chains [13] 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 [11]. This fragile nature of the $\mathcal{PT}$-symmetric phase precludes effects such as the Anderson localization [14], impurity-bound states [15], and the Luttinger-liquid behavior [16] in such a chain with a non-Hermitian Hamiltonian.

In this Rapid Communication, 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 [17].

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

$$H_{\mathcal{PT}} = -\sum_{i=1}^{N-1}(t_i c_{i+1}^{\dagger} c_i + t_{N-i}^{*} c_i^{\dagger} c_{i+1}), \tag{1}$$

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 $\langle m|\mathcal{P}|n\rangle = \delta_{m,N+1-n} = \delta_{m,\bar{n}}$, 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 $H_{\mathcal{PT}}$, 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 $H_{\mathcal{PT}}$ is purely real when the hopping elements have the same sign; in the following, we analytically derive the criteria that guarantee this robustness.

Let us consider a similarity transformation [4] of the non-Hermitian Hamiltonian, $H_{\mathcal{PT}} \to H = M^{-1} H_{\mathcal{PT}} M$, where $M = \mathrm{diag}(m_1, \ldots, m_N)$ is a diagonal matrix. It is straightforward to show that the transformed matrix H is Hermitian, $H = H^{\dagger}$, if and only if

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

We note that this constraint only applies to a diagonal M. Thus, the $\mathcal{PT}$-symmetric Hamiltonian $H_{\mathcal{PT}}$ 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 $H_{\mathcal{PT}}$ is purely real, as long as these general requirements are satisfied. Since $H = M^{-1}H_{\mathcal{PT}}M = H^{\dagger}$, it follows that the eigenvalues E_n of H and $H_{\mathcal{PT}}$ are the same, and that the orthogonal eigenvectors of H, $H|v_n\rangle = E_n|v_n\rangle$, and the (nonorthogonal) eigenvectors of the $\mathcal{PT}$-symmetric Hamiltonian, $H_{\mathcal{PT}}|u_n\rangle = E_n|u_n\rangle$ 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 $H_{\mathcal{PT}}$ are orthonormalized. We note this transformation corresponds to the positive-definite, self-adjoint, invertible metric $\eta^{-1} = MM^{\dagger}$ [13].

The hopping amplitudes for atomic orbitals can be, in general, complex [18]. However, for optical lattices, coupled waveguides, or superlattices, the hopping amplitude, determined by the overlap of adjacent on-site (Gaussian or exponential) ground-state wave functions, is positive [18]. A truly non-Hermitian Hamiltonian $H_{\mathcal{PT}}$ may be realized in systems with asymmetrical hopping due to an in-plane field or a voltage bias [19]. Its Hermitian counterpart H, with position-dependent, parity symmetric hopping, may be realized in evanescently coupled waveguides where the wave-packet evolution and two-particle quantum correlations are exquisitely sensitive to the hopping [17].

Note that Eq. (2), although dependent upon the underlying Hamiltonian $H_{\mathcal{PT}}$, 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 $H_{\mathcal{PT}}$, in numerical calculations we use its Hermitian counterpart H with entries

$$H_{mn} = -|t_m t_{N-m}|^{1/2}(\delta_{m,n-1}e^{i\theta_m} + \delta_{m-1,n}e^{-i\theta_{N-n}}), \qquad (3)$$

where we recall that $\theta_{N-n} = \theta_n$. In the following, we discuss basic properties of such a chain, with focus on the energy spectrum and nature of wave functions 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 $t_k = t_0 k^{\alpha}$, 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-hand 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 dotted-dashed line). As is expected for a tight-binding model, the energy spectra are symmetric around zero [20]. *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-hand 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 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

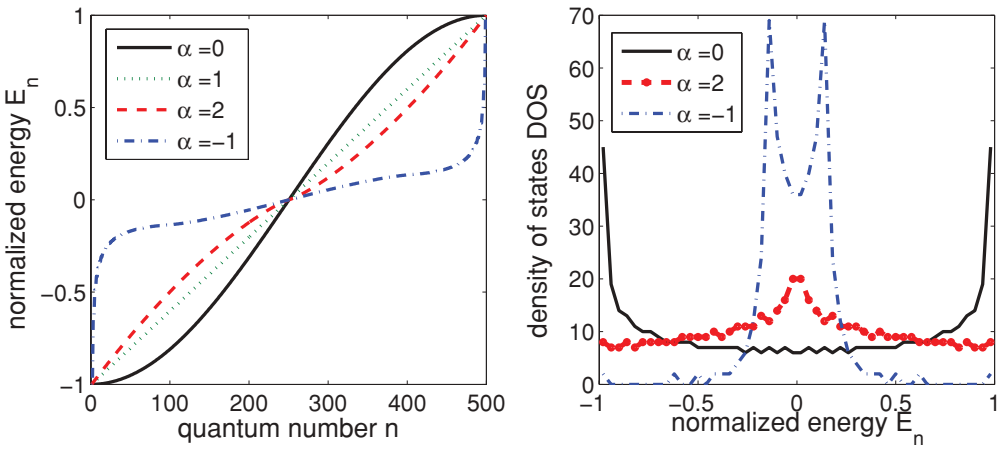

FIG. 1. (Color online) (a) The left-hand panel shows energy spectra for the robust $\mathcal{PT}$-symmetric chain, Eq. (1), with $N = 500$ sites and a position-dependent hopping amplitude $t_k = t_0 k^{\alpha}$ with $\alpha = \{0, 1, 2, -1\}$. The energy is normalized by its maximum value. When $\alpha = 0$ (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 dotted-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) The right-hand 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 dotted-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 α.

$\pm E_0 = \pm(N-1)t_0$ 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 $|\psi_\gamma\rangle = \sum_{k=1}^{N} f_k^\gamma |k\rangle$ of $H_{\mathcal{PT}}$ is

$$-t_0\left[k f_{k+1}^\gamma + (N+1-k) f_{k-1}^\gamma\right] = E_\gamma f_k^\gamma. \tag{4}$$

It is easy to check that $f_k^G = C_{k-1}^{N-1} = (N-1)!/(k-1)!(N-k)!$ satisfies Eq. (4) with eigenvalue $E_G = -(N-1)t_0$. Thus the ground-state wave function is $|\psi_G\rangle = \sum_{i=1}^{N} f_k^G |k\rangle$. Note that for $k \sim N/2 \gg 1$, the Stirling approximation implies that the ground-state wave function is Gaussian near the center of the chain, $f_k^G \sim \exp[-(k-N/2)^2/2N^2]$. The first excited-state wave function is given by $f_k^1 = (N+1-2k) f_k^G$. It has an energy $-(N-3)t_0$, and the Stirling approximation shows that in the large N limit, it carries over to the wave function 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: $f_k \to (-1)^k f_k$ [20].

When $\alpha \neq \{0,1\}$ an analytical solution for the eigenvalue spectrum $H_{\mathcal{PT}}$, or equivalently H, is unknown. However, the results in Fig. 1 for $\alpha > 0$ can be qualitatively understood with the simplest example of a nontrivial, 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 $H_{\mathcal{PT}}$ of a five-site chain with hopping parameters $\{t_1,t_2,t_3,t_4\}$ with $a = -\sqrt{t_1 t_4}$ and $b = -\sqrt{t_2 t_3}$. 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 wave functions: 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 normalized wave function $|\psi\rangle = \sum_{i=1}^{N} f_i |i\rangle$ with increasing system size N, we calculate the inverse participation ratio (R) [21]

$$R_\psi(N) = \sum_{i=1}^{N} |f_i|^4. \tag{5}$$

If the R remains finite as $N \to \infty$, the wave function is localized whereas for an extended state, $R(N) \propto 1/N^\eta \to 0$, where $\eta > 0$; for a uniform tight-binding chain, $\alpha = 0$, the $R(N) = 3/N$ for *all eigenstates*. Note that the Rs for eigenstates with energies $\pm E$ are the same. The left-hand panel in Fig. 2 shows the evolution of the maximum and minimum values of R for a chain with $N = 10$–5000 as a function of $\alpha \geqslant 0$. Note that since the chain size and the Rs span decades, we use the logarithmic scale in Fig. 2. When $\alpha = 0$ (black solid circles) we obtain the analytical result, $R(N) = 3/N$. When $\alpha > 0$, we see that both the minimum and maximum Rs decay with increasing chain size, $\max R \propto N^{-\eta_\alpha}$ and $\min R \propto N^{-\gamma_\alpha}$, where $0 < \eta_\alpha < \gamma_\alpha < 1$, and both exponents η_α and γ_α are monotonically decreasing functions of α. 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 $\alpha \geqslant 0$. The right-hand panel shows corresponding results for $\alpha \leqslant 0$. The minimum R is essentially independent of α. On the other hand, in sharp contrast with the previous results, we see that the maximum R 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

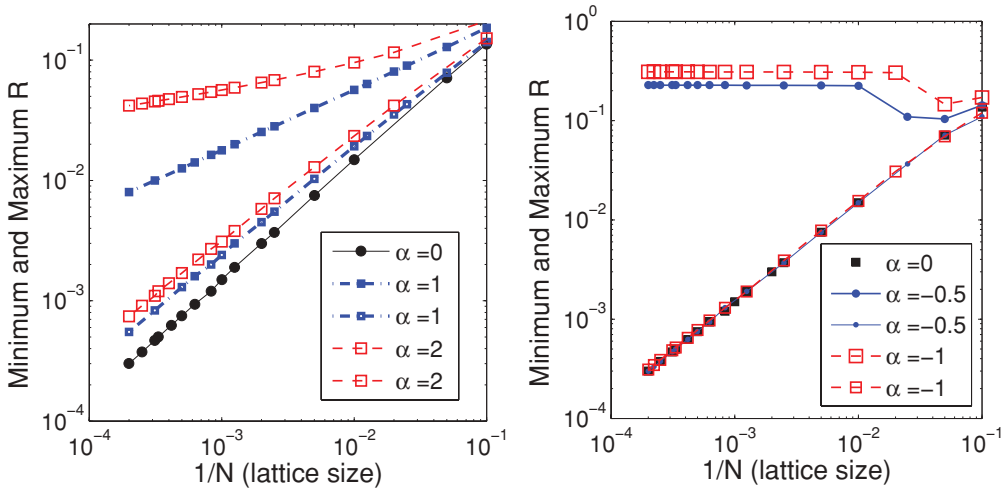

FIG. 2. (Color online) (a) The left-hand panel shows the minimum and maximum values of inverse-participation ratio (R) for an N-site chain with Hamiltonian H, Eq. (3), as a function of position-dependent hopping $t_k = t_0 k^\alpha$. When $\alpha = 0$ (black solid circles), we obtain the analytical result $R(N) \propto 1/N$. The $\alpha = 1$ (blue dotted-dashed line) and $\alpha = 2$ (red dashed line) results show that the Rs decrease monotonically with increasing chain size. These results strongly suggest that all eigenstates are extended when $\alpha \geqslant 0$. (b) The right-hand panel shows the R results for $\alpha \leqslant 0$. The $\alpha = -1/2$ (blue solid circles) and $\alpha = -1$ (red open squares) results show that the minimum R is essentially independent of α. The maximum R 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.

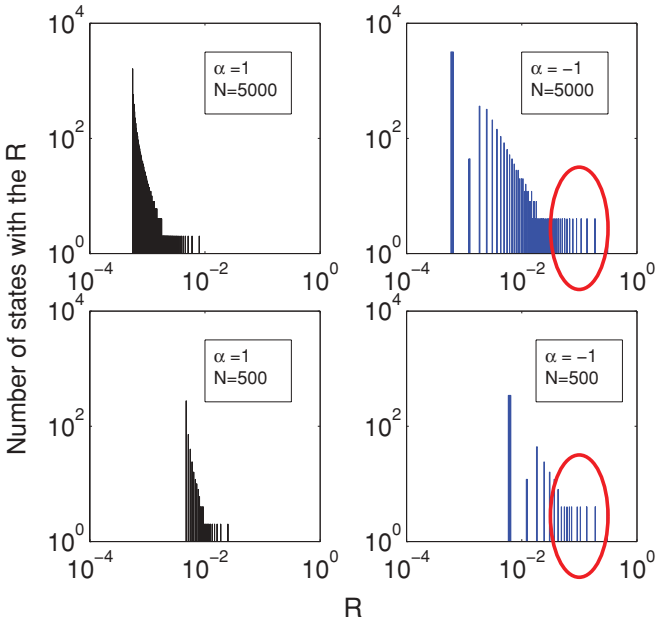

FIG. 3. (Color online) The evolution of the inverse-participation-ratio (R) distribution with the chain size N. Note the logarithmic scale. The top left-hand and bottom left-hand panels show that when $\alpha = 1$, as N increases, the entire distribution of Rs shifts to lower values. It suggests that all eigenstates of the Hamiltonian H, Eq. (3), are extended in the absence of disorder. The top right-hand and bottom right-hand panels show that when $\alpha = -1$, as N is increased, although most of the Rs 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 R is fourfold degenerate. Thus, when $\alpha < 0$, the system has both extended and localized eigenstates in the absence of disorder.

degenerate in energy; so are their staggered counterparts [20]. Thus, there are at least four eigenstates that have the same nonzero R. 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 $\sim t_0/N^{|\alpha|/2}$ at the edges to $\sim t_0/N^{|\alpha|}$ at its center.

A better insight into the number of localized states is provided by the dependence of the R distribution on the size N of the chain. Figure 3 shows the histogram of Rs for $\alpha = 1$ (left-hand column) and $\alpha = -1$ (right-hand column). When $\alpha = 1$, as N is increased tenfold from $N = 500$ (bottom left-hand panel) to $N = 5000$ (top left-hand panel), the entire R distribution shifts to smaller values. In contrast, when $\alpha = -1$, even as N is increased tenfold, the R values for a few (localized edge) states, indicated by the red oval, are unchanged while the Rs 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 [11]. In this Rapid Communication, 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) [17]. 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 α. 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 [14,21]. Thus, the physics of the robust $\mathcal{PT}$-symmetric chain with non-Hermitian hopping is extremely rich.

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