Robust and fragile $\mathcal{PT}$-symmetric phases in a tight-binding chain

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Abstract

We study the phase-diagram of a parity and time-reversal ($\mathcal{PT}$) symmetric tight-binding chain with $N$ sites and hopping energy $J$, in the presence of two impurities with imaginary potentials $\pm i\gamma$ located at arbitrary ($\mathcal{P}$-symmetric) positions $(m, \bar{m} = N + 1 - m)$ on the chain where $m \leq N/2$. We find that except in the two special cases where impurities are either the farthest or the closest, the $\mathcal{PT}$-symmetric region - defined as the region in which all energy eigenvalues are real - is algebraically fragile. We analytically and numerically obtain the critical impurity potential $\gamma_{\mathcal{PT}}$ and show that $\gamma_{\mathcal{PT}} \propto 1/N \to 0$ as $N \to \infty$ except in the two special cases. When the $\mathcal{PT}$ symmetry is spontaneously broken, we find that the maximum number of complex eigenvalues is given by $2m$. When the two impurities are the closest, we show that the critical impurity strength $\gamma_{\mathcal{PT}}$ in the limit $N \to \infty$ approaches $J(J/2)$ provided that $N$ is even (odd). For an even $N$ the $\mathcal{PT}$ symmetry is maximally broken whereas for an odd $N$, it is sequentially broken. Our results show that the phase-diagram of a $\mathcal{PT}$-symmetric tight-binding chain is extremely rich and that, in the continuum limit, this model may give rise to new $\mathcal{PT}$-symmetric Hamiltonians.
Introduction: Lattice models, including tight-binding chains, have been a cornerstone of theoretical explorations due to their analytical and numerical tractability [1], the absence of divergences associated with the ultraviolet cutoff [2, 3], the availability of exact solutions [4], and the ability to capture counter-intuitive physical phenomena including the bound-states in repulsive potentials [5]. In recent years, sophisticated optical lattice systems have increasingly permitted the experimental exploration of lattice models [6, 7]. These lattice models are largely based on a Hermitian Hamiltonian. Over the past decade, it has become clear that non-Hermitian Hamiltonians with $\mathcal{PT}$-symmetry can have purely real energy spectra [8, 9] and that, when they do, with an appropriately re-defined inner product, their eigenvectors can be appropriately orthonormalized [10]. The theoretical work has been accompanied, most recently, by experiments in optical physics where spontaneous $\mathcal{PT}$ symmetry breaking in a classical system has been observed in waveguides with $\mathcal{PT}$ symmetric complex refractive index [11]. In recent years, lattice models with a $\mathcal{PT}$ symmetric non-Hermitian “hopping” between adjacent levels of a simple-Harmonic oscillator [12], tridiagonal $\mathcal{PT}$-symmetric models [13], and tight-binding models with a Hermitian hopping and $\mathcal{PT}$-symmetric complex on-site potential [14–16] have been investigated. These models are of physical interest because they lead to unitary scattering even in the absence of a Hermitian Hamiltonian [17].

In this paper, we analytically and numerically investigate the phase-diagram of a one-dimensional tight-binding chain with hopping energy $J$ and two imaginary potentials $\pm i\gamma$ as a function of the size of the chain $N$ and the positions of the two impurities within the chain $(m, \bar{m})$ [16, 17]. Our main results are as follows: i) We show that except in the two special cases (the impurities are the closest or the farthest), in the thermodynamic limit $N \to \infty$, the critical potential strength vanishes, $\gamma_{\mathcal{PT}}(\mu) \propto 1/N \to 0$ where $\mu = m/N \leq 0.5$ is the relative position of the impurity. Thus, for a generic impurity location, the $\mathcal{PT}$-symmetric phase in this system is algebraically fragile [18]. ii) The “degree of $\mathcal{PT}$ symmetry breaking”, defined as the fraction of eigenvalues that become complex, is given by $2\mu$. iii) When the impurities are the closest, the critical potential strength is given by $\gamma_{\mathcal{PT}}(\mu = 0.5) = J$ when $N$ is even and when $N$ is odd, $\gamma_{\mathcal{PT}}(\mu \sim 0.5) \to J/2$ as $N \to \infty$. iv) By considering the continuum limit of this problem, we argue that the $\mathcal{PT}$-symmetric chain maps onto a $\mathcal{PT}$-symmetric continuum Hamiltonian with an imaginary viscous drag term.

Tight-binding Model: We start with the Hamiltonian for an $N$-site tight-binding chain with
$J > 0$ and two impurities with imaginary potentials at sites $(m, \bar{m} = N + 1 - m)$,

$$
\hat{H} = -J \sum_{n=1}^{N} \left( c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + i\gamma \left( c_m^\dagger c_m - c_{\bar{m}}^\dagger c_{\bar{m}} \right),
$$

(1)

where $c_n^\dagger (c_n)$ is the creation (annihilation) operator at site $n$, $m \leq N/2$ and $\bar{m} = (N + 1 - m) > N/2$ is the reflection-counterpart of site $m$. We only consider the single-particle sector and, since periodic-boundary conditions are incompatible with the parity operator, our system has open boundary conditions. In the lattice model, the action of the parity operator is given by $P c_n^\dagger P = c_{\bar{n}}^\dagger$ with $\bar{n} = (N + 1 - n)$, and the action of the anti-linear time-reversal operator is given by $T i T = -i$. The potential term in the Hamiltonian, Eq.(1), is odd under individual $P$ and $T$ operations, and hence the Hamiltonian is $PT$-symmetric.

The phase-diagram of this system with the impurities at the end and its equivalent Hermitian counterpart have been investigated in detail [15].

A general single-particle eigenfunction of the Hamiltonian can be written as $|\psi_k\rangle = \sum_{n=1}^{N} \psi_n^k c_n^\dagger |0\rangle = \sum_n \psi_n^k |n\rangle$ where, according to the Bethe ansatz, the coefficients $\psi_n^k$ have the form

$$
\psi_n^k = \begin{cases} 
A \sin(kn) & n \leq m, \\
P \sin(kn) + Q \cos(kn) & m < n < \bar{m}, \\
B \sin(k\bar{n}) & n \geq \bar{m}.
\end{cases}
$$

(2)

Note that open-boundary conditions, along with the requirement $\hat{H}|\psi_k\rangle = E_k|\psi_k\rangle$, constrain the eigenfunction coefficients to a sinusoidal form in the regions $n \leq m$ and $n \geq \bar{m}$ and give $E_k = -2J \cos(k)$. By considering the eigenvalue equation at points $n = m, m + 1$ and their reflection-counterparts, we find that the quasimomenta $k$ obey the equation

$$
M(k) \equiv \left[ \sin^2(k(m+1)) + \left( \frac{\gamma^2}{J^2} \right) \sin^2(km) \right] \sin(k(N-2m+1)) \\
+ \sin^2(km) \sin(k(N-2m-1)) - 2 \sin(km) \sin(k(m+1)) \sin(k(N-2m)) = 0
$$

(3)

The $PT$ symmetry is unbroken provided that Eq.(3) has $N$ real solutions. When $\gamma = 0$, the $N$ distinct solutions are given by the well-known result for a tight-binding chain with open boundary conditions, $k_\alpha = \alpha \pi/(N+1)$ where $\alpha = 1, \ldots, N$. Since $M(\pi - k) = (-1)^N M(k)$, if $k_0$ is a solution of Eq.(3), then so is $(\pi - k_0)$. It also follows that when $N$ is odd, $k = \pi/2$ is a solution irrespective of the value of $\gamma$, and that the corresponding eigenvector has zero energy. When $m = 1$, Eq.(3) reduces to the criterion for quasimomentum obtained in
Ref. [15]; in that case, as $\gamma/J \to 1$, the two central $k_\alpha \sim \pi/2$ become degenerate, the $\mathcal{PT}$ symmetry is spontaneously broken, and the system develops $N-2$ real and two complex (conjugate) eigenvalues.

FIG. 1. (color online) (a) Left panel shows the permitted values of quasimomenta $k/\pi$ as a function of impurity potential $(\gamma/J)^2$ for a chain with $N = 20$ sites and one impurity at $m = 4$ ($\mu = 0.2$, thin solid red) or at $m = 8$ ($\mu = 0.4$, thick dashed blue). The plot is symmetric about $k = \pi/2$. As $(\gamma/J)^2$ is increased, the adjacent quasimomenta $k_1 \sim \pi/(N+1)$ and $k_2 \sim 2\pi/(N+1)$ become degenerate (as do their counterparts near $k \sim \pi$) and lead to the $\mathcal{PT}$ symmetry breaking. (b) Right panel shows the critical potential strength $\gamma_{PT}(\mu)/J$ as a function of the chain size $N$ for various positions $m = \mu N$ of the impurity potential. We see that $\gamma_{PT}(\mu)$ vanishes as $N \to \infty$; thus the $\mathcal{PT}$-symmetric phase is algebraically fragile except when the impurities are either closest to each other or the farthest.

The left panel in Fig. 1 shows the typical plot of quasimomentum values $k(\gamma)/\pi$ as a function of $\gamma$, for a chain with $N = 20$ sites and the first impurity at $m=4$ (thin solid red) or $m= 8$ (thick dashed blue). Since the plot is symmetric about $k = \pi/2$, we focus only on the left-half $k/\pi \leq 0.5$ and note that since $N$ is even, there is no solution present at $k = \pi/2$. As the impurity potential $\gamma$ is increased, the adjacent quasimomenta and the corresponding energy levels become degenerate, leading to the $\mathcal{PT}$ symmetry breaking [14, 15]. We see that the critical potential for $m = 4$ is greater than that for $m = 8$, $\gamma_{PT}(\mu = 0.2) > \gamma_{PT}(\mu = 0.4)$ and, in contrast with the $m = 1$ case, the two levels that become degenerate occur in a pair, with one near the origin $k \sim \pi/(N+1)$ and other near the zone-boundary $k \sim N\pi/(N+1)$. 
Therefore when $\gamma(\mu) = \gamma_{PT}(\mu) + 0^+$, there are four complex eigenvalues. Since the $\mathcal{PT}$ symmetry breaking can be associated with the development of dissipative channels, we define the “degree of $\mathcal{PT}$-symmetry breaking” as the fraction of eigenvalues that become complex. For a general $m$, as $\gamma$ is increased beyond $\gamma_{PT}$, we find that a total of $2m$ complex eigenvalues emerge and thus the degree of $\mathcal{PT}$-symmetry breaking is given by $2\mu \leq 1$. The right panel in Fig. 1 shows the typical evolution of critical potential strength $\gamma_{PT}(\mu)$ with $N$, for $\mu = 0.2, 0.25, 0.4$, obtained by numerically solving Eq. (3). The scaling suggests that the critical potential strength for the infinite chain approaches zero, $\gamma_{PT}(\mu) \propto 1/N \rightarrow 0$. Thus, the $\mathcal{PT}$-symmetric phase, which exists in the region $0 \leq \gamma \leq \gamma_{PT}$, is algebraically fragile.

Closest Impurities and the Even-Odd Effect: We now consider the case of closest impurities. Note that due to the $\mathcal{PT}$-symmetric requirement, when $N$ is even the impurities are nearest neighbors with $m = N/2$, whereas when $N$ is odd the impurities are next-nearest-neighbors with $m = (N - 1)/2$. We will first focus on the case with an even $N$. In this case, the condition $M(k) = 0$ from Eq. (3) reduces to the following equation

$$J^2 \sin^2 \left[ k \left( \frac{N}{2} + 1 \right) \right] = (J^2 - \gamma^2) \sin^2 \left( \frac{kN}{2} \right).$$

When $\gamma = 0$ Eq. (4) has $N$ distinct solutions given by $k_\alpha = \alpha \pi / (N + 1)$. As $\gamma$ increases the adjacent $k_\alpha$ approach each other and when $\gamma = J$, Eq. (4) has $N/2$ doubly-degenerate solutions given by $k_n = 2n\pi / (N + 2)$ where $n = 1, \ldots, (N/2)$. When $\gamma > J$, it is clear that Eq. (4) has no real solutions. Thus, the $\mathcal{PT}$ symmetry is maximally broken and all $N$ eigenvalues simultaneously become complex. When $N$ is odd, the impurities are at sites $N_0 \pm 1$ where $N_0 = (N + 1)/2$ is the site at the center of the chain. The equation $M(k) = 0$ then reduces to

$$\cos(k) \left[ \sin^2(kN_0) + \left( \frac{\gamma^2}{J^2} \right) \sin^2(k(N_0 - 1)) \right] = \sin(kN_0) \sin(k(N_0 - 1)).$$


This equation has all real solutions provided \( \gamma/J \leq 1/(2 \cos k_d) \) where \( \pi/(N+1) < k_d < 2\pi/(N+1) \) corresponds to the first degenerate quasimomentum. Therefore, we find that as \( \gamma \) is increased from zero the \( \mathcal{PT} \)-symmetry breaks at \( \gamma_{PT} = J/2 \) in the limit \( N \to \infty \) when adjacent \( k_\alpha \) near the origin (and their counterparts near the zone boundary) become degenerate. Hence, for \( \gamma = \gamma_{PT} + 0^+ \), there are four complex eigenvalues. On the other hand, Eq.(5) has only one real solution, \( k = \pi/2 \), when \( \gamma/J > 1/(2 \cos k_D) \) where \( k_D \lesssim \pi/2 \) is the degenerate quasimomentum closest to the zone center \( k = \pi/2 \). Hence, the number of complex eigenvalues increases monotonically and when \( \gamma > J/(2 \cos k_D) \sim J(N+1)/3\pi \), it saturates to \( 2m = N-1 \) [19]. Figure 2 shows the quasimomenta \( k_\alpha(\gamma) \) for a chain with \( N = 13 \) and \( N = 21 \) lattice sites obtained from Eq.(5), and confirms these results. Since the \( \mathcal{PT} \) symmetric nature of the potential dictates the minimum distance between the impurities when \( N \) is odd or even, the phase-diagram of the chain is sensitive to it even as \( N \to \infty \).

**FIG. 2.** (color online) Permitted quasimomenta \( k(\gamma)/\pi \) for a chain with \( N = 21 \) (thick dotted red) and \( N = 13 \) (thin solid blue) sites as a function of impurity strength \( (\gamma/J)^2 \) when the impurities are closest to each other. As \( \gamma \) is increased, adjacent quasimomenta become degenerate leading to a spontaneous \( \mathcal{PT} \)-symmetry breaking. As \( N \to \infty \), we find that the critical potential strength \( \gamma_{PT} \to J/2 \).

**Numerical Results:** We start this section with results for the critical potential strength \( \gamma_{PT}(\mu) \) as a function of the relative impurity site location \( 0 < \mu = m/N \leq 1/2 \) obtained by numerical diagonalization of the Hamiltonian Eq.(1) for various lattice sizes \( N \), even
and odd. The left panel in Fig. 3 shows that, for an even $N$, apart from finite-size effects that are prominent near $\mu = 1/4$ and are also present in solutions to Eq. (3), the critical potential strength $\gamma_{PT}(\mu)$ is vanishingly small except at $\mu = 1/N$ and $\mu = 0.5$. In both special cases $\gamma_{PT} = J$. The right panel in the same figure shows results for odd $N$. When $\mu = 1/N$ or equivalently $m = 1$, we recover the result $\gamma_{PT} = J\sqrt{1+1/N}$ [15]. As in the case with even $N$, we find that $\gamma_{PT}(\mu)$ is suppressed with increasing $N$ everywhere except when $\mu = 0.5 - 1/2N$ or equivalently $m = (N - 1)/2$. These results are consistent with those obtained through the analytical treatment earlier.

![Fig. 3](image)

**FIG. 3.** (color online) (a) Left panel shows the critical potential strength $\gamma_{PT}/J$ as a function of the location $\mu = m/N \leq 1/2$ of the first impurity obtained via numerical diagonalization for a chain with even $N$. Except at the end-points, $\mu = 1/N$ and $\mu = 0.5$, as $N$ increases $\gamma_{PT}(\mu)$ decreases. At the end points, we find that $\gamma_{PT} = J$ is independent of the value of $N$. (b) The right panel presents similar results for an odd $N$, showing that the critical $\gamma_{PT}(\mu) \propto 1/N$ for all values of $\mu$ except for $\mu = 1/N$ and $\mu = 0.5 - 1/2N$. When $\mu = 1/N$, we recover the result $\gamma_{PT} = J\sqrt{1+1/N}$ [15], and when the impurities are next-nearest-neighbors, we find that the critical potential strength $\gamma_{PT} \to J/2$ as $N \to \infty$.

We now briefly explore the change in a (typical) eigenfunction $\psi_k(n)$ as a function of impurity potential $\gamma$ in the case of nearest-neighbor impurities (even $N$). In the $\mathcal{PT}$-symmetric phase, an eigenfunction is given by $\psi_<(n) = A \sin(ka)$ for $n \leq N/2$ and $\psi_>(n) = B \sin(k\bar{n})$ for $n > N/2$ where $k$ is a quasimomentum that satisfies Eq.(4). Using the eigenfunction constraints and Eq.(4), it follows that

$$B = A \left[ \frac{\sin(k(1+N/2))}{\sin(kN/2)} + i\frac{\gamma}{J} \right] = A \exp(i\theta_\gamma) ,$$

(6)
where the angle $\theta_\gamma$ satisfies $\tan \theta_\gamma = \gamma \sin(kN/2)/J \sin[k(1 + N/2)]$. Figure 4 shows the amplitude $|\psi_k(n)|$ and the phase $\Phi(n)$ of the ground-state wavefunction of a chain with $N = 20$ sites and nearest-neighbor impurities. The top (blue) panel shows that when $\gamma = \gamma_{PT} = J$, the wavefunction amplitude is even about the center of the chain and the phase is given by $\theta_\gamma = \pi/2$, as is expected from Eq. (6). The bottom (red) panel shows that when $\gamma = 1.01J > \gamma_{PT}/J$, the broken $\mathcal{PT}$-symmetry is reflected in the asymmetrical wavefunction amplitudes and in the position-dependent phase factor $\Phi(n)$. These are generic features of the broken $\mathcal{PT}$-symmetry phase. We also note that in the continuum limit, the eigenfunction $\psi_k(x)$ becomes discontinuous at the center of the chain while the probability amplitude $|\psi_k(x)|$ remains continuous.

**Conclusion:** We have investigated the phase diagram of an $N$-site one-dimensional chain with a pair of complex $\mathcal{PT}$-symmetric impurities located at sites $(m, \bar{m})$ within it. A remarkable feature of such a Hamiltonian, in contrast to a tridiagonal Hamiltonian with real entries [12], is that in the $\mathcal{PT}$-symmetric region, its spectrum remains confined within the energy band $\pm 2J$ of the model in the absence of impurities; as the impurity potential $\gamma$ is increased, the level spacing between adjacent energy levels decreases. Our results show that the $\mathcal{PT}$-symmetric phase of such a chain is algebraically fragile except when the impurities are farthest from each other or are closest to each other. In the latter case, we find that the $\mathcal{PT}$-symmetric phase survives when $\gamma \leq \gamma_{PT} = J$ (even $N$) or $\gamma \leq \gamma_{PT} = J/2$ (odd $N$). We note that such a chain offers tremendous tunability due to its variable critical impurity strength $\gamma_{PT}(\mu)$ for a finite $N$, and the corresponding variable fraction of complex eigenvalues $2\mu$ which translates into the number of dissipative channels in both classical [11] and quantum systems. Thus, a physical realization of such a model [16] may offer the ability to engineer the level-spacings and the dissipation in this system.

We conclude by briefly pointing out the continuum limit of this system. In the continuum limit, the lattice spacing $a$ vanishes and the number of lattice sites $N$ diverges such that the length of the chain $L = Na$ remains constant. Note that since $\sum_j (V_{PT}\psi_j)(j)$ is a constant, where $V_{PT}$ is the $\mathcal{PT}$-symmetric potential, the corresponding continuum Schrödinger eigenvalue equation is given by

$$-rac{d^2}{dx^2}\psi_k(x) - i\Gamma \delta(x) \frac{d}{dx}\psi_k(x) = k^2 \psi_k(x), \quad (7)$$

where the dimensionless impurity strength $\Gamma = \gamma/J$ for nearest-neighbor impurities (even
FIG. 4. (color online) The top (blue) panel shows the amplitude $|\psi_k(n)|$ (left) and the phase $\Phi(n)/\pi$ (right) of the ground-state wavefunction of a $\mathcal{PT}$-symmetric chain with $N = 20$ sites and nearest-neighbor impurities with strength $\gamma = \gamma_{PT} = J$. As expected of a $\mathcal{PT}$-symmetric state, the amplitude is even around the center of the chain, and the effect of a non-zero $\gamma$ is manifest in the discontinuous change in the phase, with $\Phi(n) = 0$ for $n \leq N/2$ and $\Phi(n) = \pi/2$ for $n > N/2$, consistent with Eq. (6). The bottom (red) panel shows the same state when $\gamma/J = 1.01$ and the $\mathcal{PT}$-symmetry is spontaneously broken. The broken symmetry is manifest in the asymmetrical wavefunction amplitude (left) and a position-dependent phase $\Phi(n)$.

$N), \Gamma = 2\gamma/J$ for next-nearest-neighbor impurities (odd $N$), and the eigenfunctions obey boundary conditions $\psi_k(x = \pm L/2) = 0$. Note that the continuum Hamiltonian is $\mathcal{PT}$-symmetric, but not Hermitian, due to the non-commuting parts, $\delta(x)$ and $-id/dx$, of the “potential” term. Our results imply that the $\mathcal{PT}$-symmetric phase of this Hamiltonian survives as long as $\Gamma \leq 1$, irrespective of whether the number of sites $N$ in the chain is odd or even. Indeed, Eq.(7) suggests a new class of $\mathcal{PT}$-symmetric Hamiltonians with a “viscous drag potential” term of the form $V = -ihf(x)d/dx$ that is not Hermitian but is $\mathcal{PT}$-symmetric provided $f(x)$ is an even function of $x$. In the lattice model, such a potential
will correspond to $\mathcal{PT}$-symmetric impurities at multiple locations. Detailed investigation of such models will improve our understanding of $\mathcal{PT}$-symmetry breaking in discrete and (classical) continuum systems, that can be realized in optical lattices and waveguides with complex refractive index, respectively [11].

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[19] This is strictly true only when $N = 4p + 1$. For $N = 4p - 1$, as $\gamma$ increases, the number of real eigenvalues reduces from $7 \to 3 \to 5 \to 1$. 