Universal Subdiffusive Behavior at Band Edges from Transfer Matrix Exceptional Points

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We discover a deep connection between parity-time symmetric optical systems and quantum transport in one-dimensional fermionic chains in a two-terminal open system setting. The spectrum of one dimensional tight-binding chain with periodic on-site potential can be obtained by casting the problem in terms of 2×2 transfer matrices. We find that these non-Hermitian matrices have a symmetry exactly analogous to the parity-time symmetry of balanced-gain-loss optical systems, and hence show analogous transitions across exceptional points. We show that the exceptional points of the transfer matrix of a unit cell correspond to the band edges of the spectrum. When connected to two zero temperature baths at two ends, this consequently leads to subdiffusive scaling of conductance with system size, with an exponent 2, if the chemical potential of the baths are equal to the band edges. We further demonstrate the existence of a dissipative quantum phase transition as the chemical potential is tuned across any band edge. Remarkably, this feature is analogous to transition across a mobility edge in quasiperiodic systems. This behavior is universal, irrespective of the details of the periodic potential and the number of bands of the underlying lattice. It, however, has no analog in absence of the baths.

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Introduction and overview of results.—It is fascinating how fundamental mathematical concepts aid in our understanding of physical phenomena across all scales. This often allows us to find deep connections between seemingly completely disparate physical situations. Here, we show how a property termed pseudo-Hermiticity of non-Hermitian matrices reveals a unique connection between balanced-gain-loss optical systems and quantum transport in fermionic chains.

The dynamics of two coupled optical cavities, one with gain and the other with loss, such that the gain and loss are perfectly balanced, is most commonly envisioned as being governed by the so-called 2×2 parity-time (PT) symmetric non-Hermitian "Hamiltonian" $\mathbf{H}_{\mathrm{PT}} = \omega_0 \mathbb{I}_2 + i\gamma\sigma_z + g\sigma_x$ [1–3]. Here, $\sigma_{x,y,z}$ are the Pauli matrices, and $\mathbb{I}_2$ is the 2×2 identity matrix. This 2×2 non-Hermitian matrix has the pseudo-Hermiticity property associated with the antilinear operator $\sigma_x\mathcal{K}$, i.e., $(\sigma_x\mathcal{K})\mathbf{H}_{\mathrm{PT}}(\sigma_x\mathcal{K})^{-1} = \mathbf{H}_{\mathrm{PT}}$, where σ_x describes the parity operator and $\mathcal{K}$ describes the time-reversal (complex conjugation) operator. Whenever a matrix has such a pseudo-Hermiticity, its eigenvalues are either purely real or occur in complex conjugate pairs [4–6]. When the eigenvalues are real, the eigenvectors are also simultaneous eigenvectors of the symmetry operator $\sigma_x\mathcal{K}$ with eigenvalue 1. This is termed "PT-symmetric regime." When the eigenvalues are complex, the eigenvectors of $\mathbf{H}_{\mathrm{PT}}$ are no longer simultaneous eigenvectors of the symmetry operator. This is termed "PT-broken regime." Transition between these two regimes occurs at $\gamma = g$, which is the exceptional point (EP), where there is a single eigenvalue ω_0 and the matrix is not diagonalizable. The dynamics drastically changes on transition across the EP, leading to interesting applications and exotic physics in both classical and quantum regimes [1–3,7–9]. This is the most paradigmatic example of symmetries of non-Hermitian matrices governing physical systems [9–31].

In this Letter, we explore the effects of a similar transition occurring in a different kind of non-Hermitian matrix that appears in scattering theory: the transfer matrix. Unlike mostly studied non-Hermitian matrices, transfer matrices do not directly govern the dynamics of the system. They instead play a fundamental role in determining the spectrum of the Hamiltonian of the system. The band structure of nearest neighbor fermionic chains with periodic on-site potentials can be obtained by casting the problem in terms of 2×2 transfer matrices [32–34]. We note that each such transfer matrix can be transformed to the form of $\mathbf{H}_{\mathrm{PT}}$ via a unitary transformation $\mathbf{U}$. Consequently, the transfer matrices have a pseudo-Hermiticity, associated with the antilinear operator $S = \mathbf{U}\sigma_x\mathcal{K}\mathbf{U}^{\dagger}$. So, similar to

$\mathbf{H}_{\rm PT}$, they show transitions across EPs from S-symmetric to S-symmetry-broken regimes.

We find that the EPs of the transfer matrix of a unit cell of the system correspond to the band edges. When the system is connected to two zero temperature baths at two ends (see Fig. 1); this, in turn, leads to a subdiffusive scaling of conductance with system size if the chemical potential μ is equal to any band edge. The subdiffusive scaling exponent is universal, irrespective of any further details of the periodic on-site potential. If μ is outside any system band, the eigenvalues of the transfer matrix are real (S-symmetric regime), which leads to lack of transport beyond a well-defined length scale. If μ is inside any system band, the eigenvalues of the transfer matrix are complex (S-symmetry-broken regime), which leads to ballistic transport. Thus, a transition across EP occurs in the transfer matrix when the chemical potential is tuned across a band edge. Correspondingly, there occurs a nonanalytic change in the zero temperature steady state transport properties of the open system, thereby causing a dissipative quantum phase transition. Our results can be summarized in Fig. 1. This transition occurring in the behavior of conductance as a function of μ at every band edge is reminiscent of localization-delocalization transitions across a mobility edge occurring in certain one dimensional quasiperiodic systems (for example, [35–40]). We discuss the similarities and the differences between them.

Tight-binding chain and transfer matrices.—We consider a fermionic nearest neighbor tight-binding chain of N sites with a periodic potential,

$$\hat{H}_S=\sum_{\ell=1}^{N}\varepsilon_\ell\hat{c}_\ell^\dagger\hat{c}_\ell+\sum_{\ell=1}^{N-1}(\hat{c}_\ell^\dagger\hat{c}_{\ell+1}+\hat{c}_{\ell+1}^\dagger\hat{c}_\ell), \tag{1}$$

where $\hat{c}_\ell$ is the fermionic annihilation operator at site ℓ of the chain, and ε_ℓ is a periodic on-site potential satisfying $\varepsilon_{\ell+q}=\varepsilon_\ell$. Here, q is the length of the unit cell and the hopping parameter is set to 1, which is therefore the unit of energy. We consider N to be an integer multiple of q. The periodic on-site potential with unit cell of length q causes the spectrum of the system to be separated into q bands. In the thermodynamic limit, using Bloch's theorem, the energy dispersion of the bands can be obtained via solving the following equation for ε [32–34]:

$$\mathrm{Tr}[\mathbf{T}_q(\varepsilon)]=2\cos k, \tag{2}$$

where k is the wave vector, $-\pi\le k\le\pi$, and $\mathbf{T}_q(\varepsilon)$ is given by [41]

$$\mathbf{T}_q(\varepsilon)=\prod_{\ell=1}^{q}\mathbf{T}^{(\ell)}(\varepsilon),\quad \mathbf{T}^{(\ell)}(\varepsilon)=\frac{\varepsilon-\varepsilon_\ell}{2}(\mathbb{I}_2+\sigma_z)-i\sigma_y. \tag{3}$$

Here, $\mathbf{T}^{(\ell)}(\varepsilon)$ is the transfer matrix for site ℓ, whereas $\mathbf{T}_q(\varepsilon)$ is the transfer matrix for a single unit cell of the lattice [41].

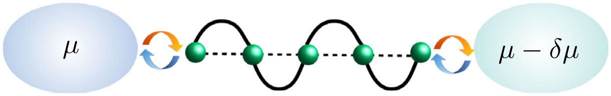
Pseudo-Hermiticity of transfer matrices.—We carry out the following unitary transformation on the transfer matrix for site ℓ, $\mathbf{U}^\dagger\mathbf{T}^{(\ell)}(\varepsilon)\mathbf{U}=[(\varepsilon-\varepsilon_\ell)/2](\mathbb{I}_2+\sigma_x)-i\sigma_z$, where $\mathbf{U}$ is the 2×2 unitary matrix that diagonalizes σ_y. The elements of $\mathbf{U}$ are $\mathbf{U}_{11}=1/\sqrt{2}$, $\mathbf{U}_{12}=1/\sqrt{2}$, $\mathbf{U}_{21}=i/\sqrt{2}$, $\mathbf{U}_{22}=-i/\sqrt{2}$. After the unitary transformation, $\mathbf{T}^{(\ell)}(\varepsilon)$ is of the exact same form as $\mathbf{H}_{\rm PT}$, and therefore commutes with $\sigma_x\mathcal{K}$. This, in turn means, $S\mathbf{T}^{(\ell)}(\varepsilon)S^{-1}=\mathbf{T}^{(\ell)}(\varepsilon)$, with $S=\mathbf{U}\sigma_x\mathcal{K}\mathbf{U}^\dagger$. Thus, transfer matrix for each site has the same pseudo-Hermiticity. Consequently, the transfer matrix of the unit cell, $\mathbf{T}_q(\varepsilon)$, which is obtained by multiplying transfer matrices for each site, also has the pseudo-Hermiticity associated with S.

The existence of the pseudo-Hermiticity guarantees that every transfer matrix has (a) a S-symmetric regime where eigenvalues are real, and eigenvectors are simultaneous eigenvectors of S and (b) a S-symmetry-broken regime where the eigenvalues are complex conjugate pairs and eigenvectors are not simultaneous eigenvectors of S. The transition between these two regimes occurs via the EP. In the following, we consider the EPs of the transfer matrix of a unit cell $\mathbf{T}_q(\varepsilon)$.

Band edges as EPs of transfer matrix of unit cell.—The band edges of the system correspond to $k=0,\pm\pi$. So, from Eq. (2), we see that the band edges $\varepsilon=\varepsilon_b$ of the system can be obtained via solution of

$$\left\{\frac{\mathrm{Tr}[\mathbf{T}_q(\varepsilon_b)]}{2}\right\}^2-1=0. \tag{4}$$

Next we note that the determinant of $\mathbf{T}^{(\ell)}(\varepsilon)$, and hence the determinant of $\mathbf{T}_q(\varepsilon)$ is 1. Using this, we can write the eigenvalues of $\mathbf{T}_q(\varepsilon)$ as $\lambda_\pm=\{(\mathrm{Tr}[\mathbf{T}_q(\varepsilon)])/2\}\pm\sqrt{\{(\mathrm{Tr}[\mathbf{T}_q(\varepsilon)])/2\}^2-1}$. From Eq. (4) we immediately



	$T_q(\mu)$	$\mathcal{G}(\mu)$
μ in system bands	$\lambda_\pm=e^{\pm ik}$ symmetry-broken regime	$\mathcal{G}(\mu)\sim N^0$ ballistic transport
μ outside system bands	$\lambda_\pm=e^{\pm\kappa}$ symmetric regime	$\mathcal{G}(\mu)\sim e^{-N/\xi}$ 'localized' localization length ξ
μ at band edges	$\lambda_\pm=1$ or -1 exceptional point	$\mathcal{G}(\mu)\sim N^{-2}$ subdiffusive transport

FIG. 1. The top panel shows a schematic of a fermionic nearest neighbor hopping chain, with a periodic on-site potential coupled at two ends to two zero temperature baths at slightly different chemical potentials, μ and $\mu-\delta\mu$. The table summarizes our main result. Here, $\mathbf{T}_q(\mu)$ is the transfer matrix of a unit cell, $\lambda_\pm$ are its eigenvalues, $\mathcal{G}(\mu)$ is the conductance in the two-terminal setting.

see that at every band edge, there is a single eigenvalue, either both 1 or both -1. Thus, every band edge corresponds to an EP of $\mathbf{T}_q(\varepsilon)$. As we discuss below, this leads to universal anomalous transport behavior at every band edge.

Quantum transport and transfer matrices.—We connect the site 1 and the site N of the lattice chain to fermionic baths, which are modeled by an infinite number of fermionic modes. The associated bath spectral functions are $\mathfrak{J}_1(\omega)$, $\mathfrak{J}_N(\omega)$. At initial time, the baths are considered to be at their respective thermal states with inverse temperature $\beta \to \infty$, and chemical potentials μ and $\mu - \delta\mu$, while the system can reside at some arbitrary initial state (see Fig. 1). We are interested in the linear response regime where $\delta\mu$ is small. As long as the bath spectral functions are continuous and the band of the bath encompass all the bands of the system, in the long time limit, the system reaches a unique nonequilibrium steady state (NESS) [42].

Using nonequilibrium Green's functions (NEGF) and the nearest neighbor nature of the system, at NESS, the zero temperature conductance can be written as [41–44]

$$\mathcal{G}(\mu) = \frac{\mathfrak{J}_1(\mu)\mathfrak{J}_N(\mu)}{2\pi|\Delta_{1,N}(\mu)|^2}, \tag{5}$$

where $\Delta_{1,N}(\mu)$ is the determinant of the inverse of the NEGF. Nearest neighbor hoppings make inverse of the NEGF tridiagonal. As a result, $\Delta_{1,N}(\mu)$ can be obtained from the following relation involving the transfer matrix [41–43]:

$$\begin{pmatrix} \Delta_{1,N}(\mu) \\ \Delta_{2,N}(\mu) \end{pmatrix} = \begin{pmatrix} 1 & -\mathbf{\Sigma}_{11}(\mu) \\ 0 & 1 \end{pmatrix} [\mathbf{T}_q(\mu)]^n \begin{pmatrix} 1 \\ \mathbf{\Sigma}_{NN}(\mu) \end{pmatrix}, \tag{6}$$

where $n = N/q$ is an integer, $\mathbf{\Sigma}_{\ell\ell}(\omega) = \int (d\omega'/2\pi) \{[\mathfrak{J}_\ell(\omega')]/(\omega - \omega')\} - i\{[\mathfrak{J}_\ell(\omega)]/2\}$, with $\ell = 1, N$, and $\Delta_{2,N}(\mu)$ is the determinant of inverse of the NEGF in absence of the first site. We immediately see from Eqs. (5) and (6) that the system-size scaling of conductance is completely independent of the type of bath spectral functions and is entirely governed by the nature of the transfer matrix $\mathbf{T}_q(\mu)$.

The system-size scaling of conductance specifies the nature of transport. In normal conductors, resistance (i.e, inverse of conductance) is proportional to length, such that resistivity is a well-defined property of the conductor. So, the behavior is $\mathcal{G}(\mu) \sim N^{-1}$ in normal diffusive transport. Departure from this behavior means resistivity is no longer a well-defined property of the material but depends on the system length. This specifies other types of transport. For ballistic transport, conductance is independent of system length, $\mathcal{G}(\mu) \sim N^0$. If $\mathcal{G}(\mu) \sim N^{-\delta}$, $\delta \neq 0, 1$, transport is said to be anomalous. For $0 < \delta < 1$, transport is called superdiffusive, while for $\delta > 1$ transport is called subdiffusive. Apart from these behaviors, conductance can decay exponentially with system length, $\mathcal{G}(\mu) \sim e^{-N/\xi}$, which shows that there is lack of transport beyond a length scale ξ. This behavior is seen in localized systems in presence of disordered or quasiperiodic potentials, with ξ being the localization length. We remark that, for anomalous transport, this classification of transport behavior does not necessarily correspond to classification of transport via spread of density correlations in an isolated system, and may lead to different results [45,46].

Universal subdiffusive scaling and dissipative quantum phase transition at every band edge.—The most remarkable result that directly follows from all of the above discussion pertains to the case where μ is equal to a band edge ε_b of the system (i.e., $|\mathrm{Tr}[\mathbf{T}_q(\mu)]| = 2$). As already noted before, the band edges of the system correspond to the EPs of the transfer matrix of a unit cell, both eigenvalues being 1. Consequently, $\mathbf{T}_q(\mu)$ cannot be diagonalized, but can be taken to the Jordan normal form via a similarity transform, $\mathbf{R}(\mu)\mathbf{T}_q(\mu)\mathbf{R}^{-1}(\mu) = \mathbb{I}_2 + (\boldsymbol{\sigma}_x + i\boldsymbol{\sigma}_y)/2$. Using properties of Pauli matrices, one then has at $\mu = \varepsilon_b$, $[\mathbf{T}_q(\mu)]^n = \mathbf{R}^{-1}(\mu)\{\mathbb{I}_2 + n[(\boldsymbol{\sigma}_x + i\boldsymbol{\sigma}_y)/2]\}\mathbf{R}(\mu)$. Note that we do not need the explicit form of $\mathbf{R}(\mu)$ to obtain this result [41]. Using this in Eq. (6), gives $\Delta_{1,N} \sim N$ for $N \gg 1$, and hence, from Eq. (5), we immediately find $\mathcal{G}(\mu) \sim N^{-2}$. Thus remarkably, because transfer matrix of a unit cell has exceptional points at every band edge, there is a universal subdiffusive scaling of conductance with system size, with a scaling exponent 2.

If μ is within the bands of the chain, then using Eq. (2) it can be shown that the eigenvalues of $\mathbf{T}_q(\mu)$ are $\lambda_\pm = e^{\pm ik}$. This corresponds to the S-symmetry-broken regime of $\mathbf{T}_q(\mu)$. The $[\mathbf{T}_q(\mu)]^n$ therefore yields an oscillatory behavior of $\Delta_{1,N}$ with N. Thus, within the bands of the chain, $\mathcal{G}(\mu)$ does not show any scaling with N, implying ballistic behavior.

On the other hand, when μ is outside the band edges of the chain, there is no solution for Eq. (2) unless k is purely imaginary ($\kappa \equiv ik$). Consequently, the eigenvalues of $\mathbf{T}_q(\mu)$ are real, and therefore corresponds to the S-symmetric regime. The eigenvalues can be written as $\lambda_\pm = e^{\pm\kappa}$, where $\mathrm{Tr}[\mathbf{T}_q(\mu)] = 2\cosh\kappa$. Since one of the eigenvalues of $\mathbf{T}_q(\mu)$ is guaranteed to have magnitude greater than 1, $\Delta_{1,N}$ diverges exponentially with system size. Consequently, $\mathcal{G}(\mu) \sim e^{-N/\xi}$, which shows lack of transport beyond a length scale ξ. The expression for ξ can be obtained as $\xi^{-1} = (2/q)\log[|\{(\mathrm{Tr}[\mathbf{T}_q(\mu)])/2\}| + \sqrt{\{(\mathrm{Tr}[\mathbf{T}_q(\mu)])/2\}^2 - 1}]$ for $|\mathrm{Tr}[\mathbf{T}_q(\mu)]| > 2$. This behavior is exactly analogous to that observed in a localized disordered or quasiperiodic system, with ξ playing the role of the localization length. In disordered or quasiperiodic systems, the finiteness of the so-called Lyapunov exponent associated with the transfer matrix is taken as the signature of localization [32,39,40,47,48]. For our setup, this quantity is given by $\ell(\mu) = \lim_{n\to\infty}(1/n)\log(||[\mathbf{T}_q(\mu)]^n||)$, where $||\mathbf{A}||$ is the norm of the matrix $\mathbf{A}$. Since one of the eigenvalues of $[\mathbf{T}_q(\mu)]^n$

diverges exponentially with n, the Lyapunov exponent is indeed finite for μ outside the system bands, and is proportional to ξ^{-1}.

Our main results are given in the table in Fig. 1. In the entire discussion above, the nature of the periodic on-site potential ε_ℓ, and its period q, which controls the number of bands, is completely arbitrary. This behavior is therefore independent of these details. As an example, we demonstrate the two-band case in Fig. 2 (see Ref. [41] for another example).

The NESS of the chain thus changes nonanalytically as a function of μ at every band edge at zero temperature. This behavior is seen in the large system-size limit, and is completely independent of the nature of bath spectral functions, as well as the strength of system-bath couplings, as long as the steady state is unique. Therefore at every band edge there occurs a dissipative quantum phase transition as a function of μ, which, in our setup, is not a Hamiltonian parameter but a thermodynamic parameter of the baths. This is unlike most other examples of dissipative phase transitions (for example, [49–63]) where a Hamiltonian parameter is changed. Like standard quantum phase transitions, this phase transition occurs strictly at zero temperature, while at finite, but low temperatures, it can be shown to manifest as a finite size crossover [41].

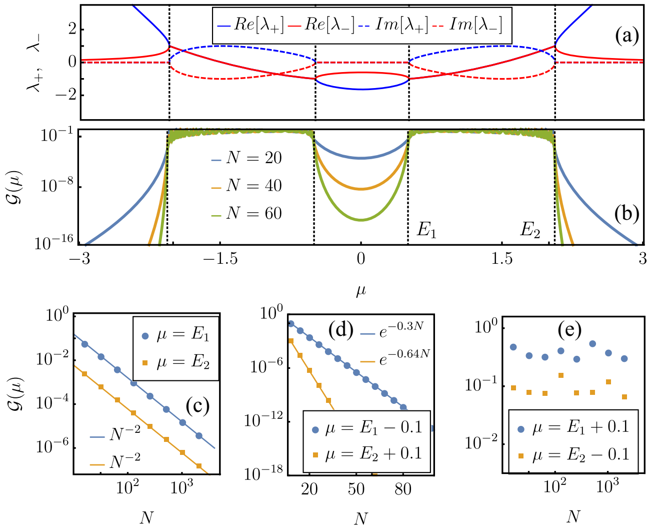


FIG. 2. (a) Real and imaginary parts of eigenvalues of $\mathbf{T}_q(\mu)$, given in Eq. (3), are plotted as a function of μ for a two-band case, i.e, $q = 2$ ($\varepsilon_l = \pm 0.5$). The vertical lines correspond to band edges [solution to Eq. (4)]. The transition across EP at each band edge is clear. (b) The zero temperature conductance $\mathcal{G}(\mu)$ vs μ is shown for three different system sizes. The nonanalytic change in system-size scaling at every band edge is clear. (c) The universal subdiffusive scaling, $\mathcal{G}(\mu) \sim N^{-2}$, is shown for μ at two chosen band edges, pointed out in panel (b). (d) The exponential decay of $\mathcal{G}(\mu)$ with N is shown for μ slightly outside the chosen band. The exponents in the fits are obtained from the formula for localization length. (e) The $\mathcal{G}(\mu) \sim N^0$ behavior is shown for μ slightly inside the chosen band. All energies are in units of system hopping strength.

Although the transition is independent of the strength of system-bath couplings, the presence of the baths is crucial. This is rooted in the fact that the mechanism for NESS transport relies not only on the chain energy states but also on the energy states available in the baths. The current-current correlations (or the associated density-density correlations) computed in absence of the baths, as often done in the Green-Kubo formalism, will not show any subdiffusive behavior for μ at band edges or the existence of a well-defined localization length for μ outside system bands. In absence of the baths, in either case, no transport is possible because all bands are either completely full or completely empty. In presence of the baths, even if there is no single particle energy eigenstate for the chain at a chosen value of μ, due to quantum nature of the particles, a small but finite probability exists for few particles to tunnel into and out of the chain, thereby making transport possible. This, in turn, leads to the exotic dissipative phase transition at every band edge. Therefore the nonanalytic change in conductance at every band edge has no obvious analog either in isolated quantum systems or in classical stochastic open systems. It also has no obvious analog in bosonic settings because Eq. (5) for conductance depends crucially on the nature of Fermi distribution at zero temperature [41].

Similarities and differences between band edges and mobility edges.—The sharp transition as a function of μ from a regime with a well-defined localization length to a regime of ballistic transport via a “critical point” showing subdiffusive scaling is akin to localization-delocalization transitions as a function of energy seen in some quasiperiodic systems (for example, [35–40,64]). The energy where this transition happens is called the mobility edge. In this sense, in a two-terminal setup, every band edge behaves like a mobility edge. A mobility edge in a two-terminal setup acts as an energy filter for quantum transport. This property can find potential applications in devising efficient autonomous thermal machines [65,66]. Since every band edge has the same effect, band edges can also be potentially used for the same purpose.

Despite the analogy between our setup and quasiperiodic systems, there are stark differences. Unlike our setup, for the quasiperiodic systems with mobility edge, the transition in conductance scaling with system size in presence of baths can be linked to a transition in nature of single-particle eigenstates of the system in absence of the baths (see, for example, [35–40,64]). This is very different from the transition observed in our setup, which is rooted in transition across EP of the transfer matrix of a unit cell. Note that, while a unit cell is well-defined for a periodic on-site potential, for quasiperiodic on-site potential, a unit cell does not exist.

Conclusions and outlook.—We have shown how non-Hermitian transitions in the transfer matrix of Hermitian

Hamiltonians affect the nature of quantum transport (see Fig. 1). In doing so, we have united two seemingly disparate concepts: (i) the symmetries and transitions in non-Hermitian matrices studied in non-Hermitian optics and (ii) band structure and quantum transport in fermionic systems studied in condensed matter and statistical physics. We find that this connection offers an extremely simple way to understand several nontrivial features of mobility edges, localization length and anomalous transport in a two-terminal open system setting, without considering disordered or quasiperiodic potentials. We discover a completely different way subdiffusive scaling of conductance, with a universal exponent, can originate: from exceptional points of transfer matrices. We remark that explaining the origin of subdiffusive scaling exponents is often a difficult problem [64,67,68].

Our results are relevant for platforms showing bands of ballistic electron transport (for example, [69–73]). They pave the way for understanding band structure and quantum transport in more exotic cases, such as higher dimensional short-ranged systems, in terms of the non-Hermitian properties of their associated transfer matrices [33,34]. But, the transfer matrix picture presented here does not hold in presence of long-range hopping. However, interestingly, the subdiffusive behavior $\mathcal{G}(\mu) \sim N^{-2}$ at band edges was also recently numerically seen in presence of long-range, power-law-decaying hopping [74]. This points to the superuniversality of this behavior at band edges, the deeper understanding of which requires further work. Investigations in these directions will be carried out in future works.

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