Measuring non-Unitarity in non-Hermitian Quantum Systems

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Non-orthogonality in non-Hermitian quantum systems generates tremendous exotic quantum phenomena, which can be fundamentally traced back to non-unitarity and is much more fundamental and universal than complex energy spectrum. In this paper, we introduce an interesting quantity (denoted as \( \eta \)) to directly and efficiently measure non-unitarity and the associated non-Hermitian physics. By tuning model parameters of underlying non-Hermitian systems, we find that the discontinuity of both \( \eta \) and its first-order derivative (denoted as \( \partial \eta \)) pronouncedly captures rich physics that is fundamentally caused by non-unitarity. More concretely, in a 1D non-Hermitian topological system, two mutually orthogonal edge states that are respectively localized on two boundaries become non-orthogonal in the vicinity of discontinuity of \( \eta \) as a function of model parameter, which is dubbed “edge state transition”. For the discontinuity of \( \partial \eta \), by investigating a two-level non-Hermitian model, we establish the connection between the points of discontinuity of \( \partial \eta \) and exceptional points (EPs), Furthermore, for models with more than two levels, we analytically obtain the upper bound of the quantity \( \eta \) with a novel dependence on the configuration of EPs. By investigating this connection in more general lattice models, we find that two concrete models at phase transition points have discontinuity of \( \partial \eta \), implying the existence of EPs, while another model constructed by the regular Sturm-Liouville theory exhibit continuous and differentiable \( \eta \) but doesn’t have an EP at the phase transition point. For more concrete applications and a systematic analytic theory about \( \eta \), we leave them for future work.

Introduction.— Recently, non-Hermitian systems [1–5] have drawn great interests, due to exotic quantum phenomena, e.g., generalized bulk-edge correspondence [6,8], exceptional points (EPs) [5, 9, 17], non-Hermitian skin effect [18, 22] and unidirectional invisibility [23]. For theoretically understanding these phenomena, non-Bloch band theory [6,8,24,29], which generalizes the conception of Brillouin zone, is established and applied to analyze the topological phase [5, 50] in non-Hermitian systems. Remarkably, non-Hermitian skin effect, the natural consequence of generalized Brillouin zone, is found to have a connection to EPs [22]. Meanwhile, compared with Hermitian systems, the classification [31,36] of topological phases in non-Hermitian systems has been significantly enriched. In addition, from the quantum-informative perspective, quantum entanglement properties of non-Hermitian systems [37–41] exhibit highly unusual features in entanglement entropy and entanglement spectrum. Besides the crystalline system mentioned before, non-Hermiticity has also been introduced to noncrystalline systems, e.g. quasi-crystal systems [41–45] and disorder systems [46–49].

While complex energy spectrum exists in many non-Hermitian systems, real energy spectrum generally holds in many systems, e.g., with \( PT \) symmetry [1, 50]. Thus, it is apparently that complex energy spectrum is not a special sign of non-Hermitian physics. In this paper, to explore physics of non-Hermitian systems, we focus the property of non-unitarity, i.e., the non-orthogonal eigenvectors [51]. When eigenvectors are not mutually orthogonal, the familiar inner product in Hermitian systems is no longer valid and the usual definition of quantum expectation of operators is no longer proper. To proceed further, in the literature, the idea of bi-orthogonal basis is introduced. More concretely, for a non-Hermitian Hamiltonian \( H \), the right eigenvectors \( |R, n \rangle \) obey \( H|R, n \rangle = E_n|R, n \rangle \), and left eigenvectors \( |L, n \rangle \) obey \( H^\dagger|L, n \rangle = E_n^\ast|L, n \rangle \), then bi-orthogonality relation can be represented as \( \langle L, n | R, m \rangle = \delta_{nm} \). When the system remains unitarity, \( \langle L, n | L, m \rangle = \langle R, n | R, m \rangle = \delta_{nm} \).

Thanks to the bi-orthogonality relation, many theoretical approaches originally introduced in Hermitian systems can be borrowed to study non-Hermitian systems. Therefore, a series of physical conceptions are reproduced in non-Hermitian systems [18, 24, 30, 52].

By using bi-orthogonal basis, we can study non-Hermitian quantum systems by constructing Hilbert space. Nevertheless, it is still unclear how to simply and efficiently characterize non-unitarity associated with the non-orthogonality among right-eigenvectors (or left-eigenvectors). To discuss non-unitarity of non-Hermitian systems, without loss of generality, we focus on studying the property of right basis but not the whole bi-orthogonal basis in this work (because left eigenvectors have the similar property with right eigenvectors). In this paper, we define a quantity to measure the strength of non-unitarity of non-Hermitian systems as follows:

\[
\eta = \frac{\sum_{n<m} |\langle R, n | R, m \rangle|^2}{\sum_{n<m} |\langle R, n | R, m \rangle||\langle R, m | R, m \rangle|},
\]

where \( 0 \leq \eta \leq 1 \). When \( \eta = 0 \), the system is unitary with mutually orthogonal eigenvectors. On the contrary, when \( \eta = 1 \), the eigenvectors are totally coalescent, resulting in the extreme case of non-unitarity.

In this paper, we apply \( \eta \) to various interesting non-Hermitian models. Then we study the behavior of the quantity \( \eta \) with the parameters of system varying. We find the various behaviors of the quantity \( \eta \), such as the discontinuity of the quantity \( \eta \) and its first-order derivative \( \partial \eta \), would imply some consequences happening in non-Hermitian systems. For example, when a non-Hermitian systems has edge...
state transition, i.e., the orthogonal edge states becoming non-orthogonal, the quantity $\eta$ would have discontinuity point. For studying the physical consequence causing the discontinuity of $\partial \eta$, we use a two-level model exhibiting that when the quantity $\eta$ near the EP, $\partial \eta$ would become discontinuous. Therefore, this feature of $\eta$ can be regarded as an evidence to identify the existence of EPs. Meanwhile, by using this feature, we infer that some non-Hermitian systems at the transition points would have EPs. Finally, we discuss the behavior of $\eta$ in a special non-Hermitian model, where this model has real energy spectrum without $\mathcal{P}\mathcal{T}$ symmetry and EPs. We find that the discontinuity of $\partial \eta$ does not appear.

The discontinuity of $\eta$.— It is known that the energy spectrum of non-Hermitian systems possesses a real-complex transition, which can be understood as a consequence of $\mathcal{P}\mathcal{T}$ symmetry breaking. To focus on the nature of non-unitarity of non-Hermitian systems, we consider the behavior of the quantity $\eta$ in a 1D non-Hermitian model [53] which always has real energy spectrum without $\mathcal{P}\mathcal{T}$ symmetry:

$$H = \sum_n \left( t_1 c_{n,A}^\dagger c_{n,B} + \frac{t_1}{g} c_{n,B}^\dagger c_{n,A} + t_2 c_{n+1,A}^\dagger c_{n,B} + \frac{t_2}{g} c_{n,B}^\dagger c_{n+1,A} \right),$$

where the operators $c_{n,A(B)}$ denote annihilation operators of spinless fermions at the sublattice A (B) in the $n$th unit cell. The real parameter $g$ is introduced to tune the system away from $g = 1$ which is the Hermitian point. In Fig. 1(a-c), we plot energy spectrum of the model (2) with open boundary condition as a function of $t_1$ with $t_2 = 1$ and three typical values of $g$. Clearly, the model (2) in both Hermitian and non-Hermitian regimes has almost identical energy spectrum and identical locations of topological phase transition, as discussed concretely in Ref. [53]. Thus, it is impossible to extract non-Hermitian effect from the energy spectrum. For this purpose, we utilize the quantity $\eta$ defined in Eq. (1) to measure non-unitarity of this model.

In Fig. 1(d-f), we study $\eta$ as a function of the parameter $t_1$ with $t_2 = 1$ and three typical values of $g$. When the parameter $g \neq 1$ in the model (2), the quantity $\eta$ as a function of $t_1$ shows exotic discontinuous points that separate upper and lower flat (“degenerate”) platforms in Fig. 1(d) and (e). In Fig. 1(f), $\eta$ is always zero and thus featureless in the Hermitian point $g = 1$. Furthermore, we find that the discontinuity points of the function $\eta$ are induced by an exotic transition of edge states. Namely, when the value of $\eta$ is located in the lower platform, two edge states are respectively localized at two endpoints of the 1D chain, as indicated by the two different colored curves in Fig. 1(g) that is obtained by taking $t_1 = 0, g = 0.5, t_2 = 1$ as an example. It is clear that the inner product of the two edge states vanishes so they are orthogonal to each other. On the other hand, when we consider $t_1 = -0.22$ that is a typical point with $\eta$ being located in the upper platform ($t_2 = 1, g = 0.5$), the amplitudes of the two edge states form the same “U-shape” distribution with maxima being simultaneously localized at two endpoints of the 1D chain, which leads to mutually non-orthogonal edge states, as shown in Fig. 1(h). This exotic non-Hermitian effect has no counterpart in topological Hermitian systems. In conclusion, while edge state transition does not show up in energy spectrum, the discontinuity of the function $\eta$ can be applied to clearly signal the transition in topological non-Hermitian systems, demonstrating the usefulness of the quantity $\eta$ in measuring non-unitarity.

The discontinuity of $\partial \eta$.— In the following, we move to the physics of discontinuity of $\partial \eta$, i.e., the first order derivative of $\eta$. For the purpose, as a warm-up, we first introduce a two-level system to study the behavior of the quantity $\eta$:

$$H_0 = \begin{pmatrix} 0 & \gamma \\ 1 & 0 \end{pmatrix},$$

where $\gamma \in \mathbb{R}$. By diagonalization, the (right)-eigenvectors of $H_0$ can be obtained and written as $(\pm \sqrt{\gamma}, 1)^T$, which results in an analytic form of $\eta$:

$$\eta = \frac{|1 - |\gamma||^2}{(1 + |\gamma|)^2}.$$  

It is apparent that when $\gamma = 1$, the model $H_0$ becomes Hermitian with $\eta = 0$. On the contrary, when $\gamma = 0$, $H_0$ reduces to
a lower triangular matrix which describes a typical EP, and the quantity \( \eta = 1 \). Next, we study the behavior of the quantity \( \eta \) as a function of \( \gamma \) near the EP. As shown in Fig. 2(a) we find that \( \eta \) at EP has a peak and its derivative (denoted as \( \partial \eta \)) is discontinuous. In the following, we will show that this feature of \( \eta \) can be regarded as an evidence to identify EPs in more general non-Hermitian quantum systems.

Since this model \([3]\) has merely two levels, the quantity \( \eta \) at EP can take the maximum value 1 and all eigenvectors are coalescent. However, for models with more than two levels, it usually has various EPs with different degeneracies. Consequently, the eigenvectors are not totally coalescent, and the value of \( \eta \) is subject to an upper bound that depends on the configuration of EPs:

\[
\eta \leq \sum_n d_n(d_n - 1) / N(N - 1) \leq 1 ,
\]

where \( N \) is the dimension of Hamiltonian matrix of non-Hermitian systems and \( n \) is the number of EPs with \( d_n \)-fold degeneracy. Only when the non-Hermitian system has one EP with \( N \)-degeneracy, the upper bound equal to 1. More detailed discussion of Eq. (5) is given in Supplemental Materials.

To illustrate the physics of the discontinuity of \( \partial \eta \), we will study two concrete non-Hermitian lattice models. Firstly, we consider a non-Hermitian quasi-crystal lattice model \([41]\) which has a localization-delocalization transition induced by non-Hermiticity:

\[
H = \sum_n \left( J_R c_n^\dagger c_{n+1} + J_L c_n^\dagger c_{n+1} \right) + \sum_n V_n c_n^\dagger c_n ,
\]

where \( c_n (c_n^\dagger) \) is the annihilation (creation) operator of spinless fermion at the \( n \)th lattice site. \( V_n = V \exp(-2\pi i \alpha n) \) is a site-dependent incommensurate complex potential parameterized by an irrational number \( \alpha \). The potential strength \( V \) is positive and real. We set the parameter \( \alpha = \sqrt{2} \approx 2.828 \) same as Ref. \([41]\). In the practical simulations, we set the length \( L = 169 \) of the system with periodic boundary condition. As discussed in Ref. \([41]\), metal-insulator phase transition (MIT) of this model \([41]\) occurs at the point \( V = 1 \). In Fig. 3 we can see that the quantity \( \eta \) as a function of \( V \) exhibits a sharp peak at \( V = 1 \), and a discontinuity point of the derivative of \( \eta \) coincides with \( V = 1 \) point. These features of \( \eta \) in the model \([41]\) are similar with the features in the two-level model \([5]\). Therefore, we infer that the model \([41]\) have EPs at the MIT transition point.

Secondly, we consider a 1D non-reciprocal Su-Schrieffer-Heeger (SSH) model \([54]\):

\[
H = \sum_n \left[ t_1 c_n^\dagger c_{n+1} + t_1 c_{n+1}^\dagger c_n + \right.
\]

\[
(t_2 + g) c_n^\dagger c_{n+1} + \left. (t_2 - g) c_n c_{n+1}^\dagger \right] ,
\]

where \( c_{n,A} (c_{n,B}) \) respectively denote annihilation operators of spinless fermions at sublattice \( A \) (B) in the \( n \)th unit cell. We restrict the parameters \( g, t_{1,2} \) in the real regime. When the parameters satisfy the condition \( |t_1| < \sqrt{t_2^2 - g^2} \), the system is in a non-Hermitian topological phase with non-trivial winding number and two edge states. When \( |t_1| > \sqrt{t_2^2 - g^2} \), the system is in a trivial phase without edge states. Thus, a topological phase transition occurs at \( |t_1| = \sqrt{t_2^2 - g^2} \), which can be identified by the appearance/disappearance of zero energy modes in Fig. 4(a). Meanwhile, we study the quantity \( \eta \) as a function of \( t_1 \) in the model \([7]\). We find the phase transition point also coincides with the discontinuity point of \( \partial \eta \) in Fig. 4(b) which is obtained from \( \eta \) in Fig. 4(b). Then, we infer that the model \([7]\) at the transition point \( |t_1| = \sqrt{t_2^2 - g^2} \) has EPs, where we take enough numerical precision for obtaining the eigenvectors of this model \([7]\). In addition, due to the existence of non-Hermitian skin effect in the model \([7]\), the derivative of \( \eta \) at the transition point suffers from finite-size effect, see more detailed discussion in Supplemental Materials.

Furthermore, we realize that this model also exhibits a significant discontinuity of \( \eta \) at \( t_1 = 0.15 \) in Fig. 4(b). Following what’s been done in the model \([2]\), we plot the edge states of the system of two parameter points \( t_1 = 0.133 \) and \( t_1 = 0.333 \) near the discontinuity point \( t_1 = 0.15 \) respectively in Fig. 4(d) and (e). We find that the edge states separately localized at two boundaries are orthogonal in Fig. 4(d), while in Fig. 4(e), the
two edge states are simultaneously localized at one boundary and become non-orthogonal \([54, 55]\). Therefore, the discontinuity of \(\eta\) in this is also induced by this edge state transition, which is similar to the physics in the model \([2]\). Moreover, it should be noted that the numerical precision of diagonalizing the Hamiltonian matrix of the model \([2]\) would influence the location of discontinuity points of \(\eta\), where this phenomenon originates from the finite-size effect.

To further investigate the connection between the discontinuity of \(\partial \eta\) and the existence of EPs, let us consider a 1D non-Hermitian model \([55]\) with topological phase transition at Hermitian point and absence of EPs:

\[
H = t_0 \sum_n \left( \frac{1}{g} b_n^\dagger a_n + ga_n^\dagger b_n + \frac{1}{g} b_{n+1}^\dagger c_n + g c_n^\dagger a_n + g a_{n+1}^\dagger c_n + g c_{n+1}^\dagger a_{n+1} \right),
\]

where \(a_n^\dagger, b_n^\dagger, c_n, c_n^\dagger\) respectively denote the annihilation(creation) operator of spinless fermions at sublattice A, B and C in the \(n^\text{th}\) unit cell. This model always has real energy spectrum without \(\mathcal{PT}\) symmetry. When the parameter \(g < 1\) \((g > 1)\), the system is trivial (topological) phase. As discussed in Ref. \([53]\), the system with non-trivial Zak phase in the parameter range \(g > 1\) has topological edge states as shown in Fig.5(a).

Keeping the critical point \(g = 1\) in mind, we study the value and derivative of \(\eta\) as the functions of the “non-Hermiticity inducer” \(g\) in the model \([55]\) as shown in Fig. 5(b) and (c). We find that \(\eta\) reaches its minimum exactly at \(g = 1\) where the derivative vanishes and the model recovers Hermiticity. Apparently, the derivative of \(\eta\) is always continuous in this model, which is different from that in the models \([6, 7]\). By careful analysis, we find this difference originates from the model construction \([55]\) of using the regular Sturm-Liouville theory \([56]\) (more discussion see Supplemental Materials). This theory guarantees the complete basis of the model \([55]\), so EP is absent in this system. Therefore, without EP, the derivative of \(\eta\) in this model \([55]\) would not have discontinuity point.

**Conclusion and outlook.**— Non-unitarity is more fundamental property than complex energy spectrum in non-Hermitian systems. To measure non-unitarity of non-Hermitian systems, we have defined a quantity \(\eta\) which locates in the interval \([0, 1]\). As an indicator of non-unitarity, the discontinuity of the quantity \(\eta\) helps us identify rich physics that has no counterpart in Hermitian quantum systems.

For the non-Hermitian lattice systems with EPs, the Hamiltonian matrix is defective matrix not having a complete basis of eigenvectors. Meanwhile, the numerical algorithm for di-
agonalizing defective matrix is not convergence\cite{57}. Therefore, it is hard to directly identify the existence of EPs. Our introduced quantity $\eta$ provides alternative route to the features of EPs, e.g., by computing the behavior of $\eta$ in the parameter space and searching discontinuity. In conclusion, we report the introduction of $\eta$ and show its efficiency and usefulness in characterizing non-Hermitian physics. For more concrete applications and a systematic analytic theory about $\eta$ (e.g., physics of the derivative of $\eta$ of all-th orders, and relation to entanglement \cite{38, 41, 58, 59}), we leave them for future work.

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SUPPLEMENTAL MATERIALS

Part-A: The upper bound of the quantity $\eta$, Jordan normal form, and EPs

In this part, we discuss the upper bound of the quantity $\eta$ in non-Hermitian lattice systems. Based on Ref. [60], due to not having a complete basis of eigenvectors, a defective matrix is not diagonalizable. However, it can be transformed to Jordan normal form with nontrivial Jordan block which describes an EP. Therefore, the non-Hermitian systems described by defective matrix has EPs.

Next, we consider the relation between the upper bound of the quantity $\eta$ and EPs. Concretely, when the EPs appear in the non-Hermitian lattice system, the Hamiltonian matrix can be transformed to Jordan normal form written as

$$ H = \begin{bmatrix} \lambda_1 & 1 \\ \lambda_1 & 1 \\ \lambda_2 & 1 \\ \lambda_2 & 1 \\ & \ddots \\ \lambda_n & 1 \end{bmatrix}, \quad (9) $$

where the model have $n$ Jordan blocks with $d_n$-fold degeneracy. Based on the property of the Jordan normal form, the eigenvectors of a Jordan block are identical. Then, a Jordan block will contribute $d_n(d_n-1)/2$ for the numerator in Eq. (1) of the quantity $\eta$. Furthermore, we sum all the contribution of all Jordan blocks for the quantity $\eta$, and the denominator in Eq. (11) of the quantity $\eta$ is $N(N-1)/2$, where $N$ is the dimension of the matrix (9). Therefore, we obtain the upper bound of the quantity $\eta$ represented as:

$$ \eta \leq \sum_n d_n(d_n-1)/N(N-1). \quad (10) $$

When the Hamiltonian matrix of non-Hermitian systems becomes defective matrix with the parameters varying, the equality of Eq. (10) is satisfied. Furthermore, from the expression of upper bound in Eq. (5), we found that the upper bound is less than 1. Meanwhile, when the system is Hermitian, the Hamiltonian matrix only have trivial jordan blocks with the dimension $d_n = 1$, therefore, the upper bound equals to 0.

Part-B: The finite-size effect of non-Hermitian SSH model (7).

Part-C: The property of a class of special models and Sturm-Liouville theory

In this part, we discuss the properties of the model (8) in main text. This model is constructed from the equation given as:

$$ H_0 \Psi_n = E_n M \Psi_n, \quad (11) $$

where $H_0$ is a Hermitian matrix, $M$ is a real diagonal matrix with diagonal element $M_{ii} > 0$. This equation is discussed in the regular Sturm-Liouville theory [56]. Meanwhile, as discussed in Ref. [53], the Hamiltonian matrix of the model (8) is represented as $M^{-1} H_0$ and non-Hermitian.

Let us review some properties of Eq. (11) to demonstrate the model in Ref. [53] having real energy spectrum. Due to the property of the regular Sturm-Liouville theory [56], 0 is not the eigenvalue of $H_0$. Then, Eq. (11) can transformed to

$$ \lambda_n M \hat{M} \hat{\Psi}_n = (M \hat{K} M \hat{z}) M \hat{z} \hat{\Psi}_n, \quad (12) $$
where $K$ is the inverse of $H_0$, and $\lambda_n = E_n^{-1}$. Furthermore, the matrix $K' = M^{\frac{1}{2}}KM^{\frac{1}{2}}$ is Hermitian, which is proven by:

$$(M^{\frac{1}{2}}KM^{\frac{1}{2}})\dagger = (M^{\frac{1}{2}})\dagger K\dagger (M^{\frac{1}{2}})\dagger = M^{\frac{1}{2}}KM^{\frac{1}{2}}. \quad (13)$$

This proof is based on the Hermitian of the matrices $K$ and $M^{\frac{1}{2}}$. Therefore, from Eq. (12), we find the eigenvalues $\lambda_n$ are real, and the eigenvalues $E_n$ of $M^{-1}H_0$ are real. Meanwhile, we find the eigenvectors $\Psi_n = M^{\frac{1}{2}}\Psi_n'$ are a set of orthogonal and complete basis satisfying the relation

$$\langle \Psi_n' | \Psi_m' \rangle = \langle \Psi_n | M | \Psi_m \rangle = \delta_{n,m}, \quad (14)$$

where $\delta_{n,m}$ is the Kronecker delta. Based on the relation (14), the eigenvectors $\Psi_n$ of the matrix $M^{-1}H_0$ are always complete. For a non-Hermitian system with EPs, the basis of eigenvectors is not complete. Then, EP is absent in the model (8).