Relationship between the Electronic Polarization and the Winding Number in Non-Hermitian Systems

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We discuss an extension of the Resta's electronic polarization to non-Hermitian systems with periodic boundary conditions. We introduce the "electronic polarization" as an expectation value of the exponential of the position operator in terms of the biorthogonal basis. We found that there appears a finite region where the polarization is zero between two topologically distinguished regions, and there is one-to-one correspondence between the polarization and the winding number which takes half-odd integers as well as integers. We demonstrate this argument in the non-Hermitian Su-Schrieffer-Heeger model.

So far, non-Hermitian quantum mechanics has been discussed for some specific situations.¹⁻⁶⁾ In recent years, this field has attracted much attention in connection with topological phases^{7,8)} due to its relevance to the open quantum systems.⁹⁻¹²⁾ The application of topology in conventional Hermitian quantum systems has relied on the principle of bulkedge (-boundary) correspondence^{13–15}) where the edge or surface states in open boundary systems can be characterized by topological invariants calculated under periodic boundary conditions (PBCs). However, it has been pointed out that such a bulk-edge correspondence may not be established in non-Hermitian systems.^{16–18)} As a result, a macroscopic number of bulk states localize at a boundary of the system which is called as the non-Hermitian skin effect. The skin effect is topologically characterized by the winding numbers defined by the non-Bloch band theory,19-21) and that defined by the Bloch Hamiltonian and the complex spectrum in open systems,²²⁻²⁶⁾ the biorthogonal polarization, $2^{7,28}$ and so on.

In this paper, inspired by these studies, we discuss the electronic polarization in non-Hermitian systems. Throughout of this paper, we consider only periodic systems, since we need to know fundamental relationship between topological quantities, before proceeding to deal with open boundary systems. For conventional Hermitian quantum lattice systems, the electronic polarization has been introduced by Resta to evaluate the expectation value of the position operator in periodic systems as $z^{(q)} = \langle \Psi_0 | e^{i(2q\pi/L)\hat{X}} | \Psi_0 \rangle$ with q = 1, where $\hat{X} = \sum_{j=1}^L \hat{x}_j$ with \hat{x}_j being the position operator at *j*-th site, *L* is the number of lattices, and $|\Psi_0\rangle$ is the ground-state many-body wave function.^{29,30)} This quantity can also be interpreted as the overlap between the ground state and a variational excited state appearing in the Lieb-Schultz-Mattis (LSM) theorem.^{31–33)} $z^{(q)}$ with $q \ge 2$ can be interpreted as extensions of the LSM theorem for general magnetizations and fillings,^{34,35)} and by later equivalent discussions.³⁶⁾ Resta related $z^{(1)}$ with the electronic polarization as $\lim_{L\to\infty} (e/2\pi)$ Im $\ln z^{(1)}$. Here and hereafter we call $z^{(q)}$ itself "polarization". The polarization $z^{(q)}$ has been calculated in various systems^{36–39)} and is shown to characterize topological phases and topological transitions in one-dimensional systems. Recently, an extension of the polarization to higher-dimensional systems has been proposed based on spiral boundary conditions.⁴⁰⁾

out that the electronic polarization in non-Hermitian systems can be related to a winding number which may take half integers.^{17,41–43)} We will demonstrate this argument in the non-Hermitian Su-Schrieffer-Heeger (SSH) model.^{19,44,45)}

We introduce the biorthogonal system. The right and left eigenstates for a 1D quadratic non-Hermitian Hamiltonian in real space satisfy the following eigenvalue equations:

$$\sum_{j'} H_{jj'} |\psi_{k\mu}^{j',\mathsf{R}}\rangle = E_{k\mu} |\psi_{k\mu}^{j,\mathsf{R}}\rangle, \qquad (1a)$$

$$\sum_{j'} H_{jj'}^{\dagger} |\psi_{k\mu}^{j',L}\rangle = E_{k\mu}^{*} |\psi_{k\mu}^{j,L}\rangle, \qquad (1b)$$

respectively, where $|\psi_{k\mu}^{j,\alpha}\rangle = \mathcal{U}_{jk}^{-1} |u_{k\mu}^{\alpha}\rangle$ ($\alpha = R, L$), μ is a band index, $\mathcal{U}_{kj} = e^{-ikx_j}/\sqrt{L}$, and $|u_{k\mu}^{\alpha}\rangle$ with the normalization condition $\langle u_{k\mu}^{L} | u_{k\nu}^{R} \rangle = \delta_{\mu\nu}$ is the eigenstate of the non-Hermitian Bloch Hamiltonian $H(k) = \sum_{jj'} \mathcal{U}_{kj} H_{jj'} \mathcal{U}_{j'k}^{-1}$.

Then we define the polarization in non-Hermitian systems as follows;

$$z^{(q)} = \langle \Psi_{\rm L} | U^q | \Psi_{\rm R} \rangle, \quad U = \exp\left[i\frac{2\pi}{L}\sum_{j=1}^L \hat{x}_j\right],$$
 (2)

where $|\Psi_{R(L)}\rangle$ is the Slater determinant constructed by the occupied right (left) eigenstate, and $\hat{x}_j = jn_j$, where n_j is the number operator of the electron at the *j*-th unit cell. The definition (2) for q = 1 was first introduced by Lee, *et al.*⁴⁶⁾ They obtained the right and left many-body ground states by numerical diagonalization in real space and calculated Im $\ln z^{(1)}$, which takes 0 or π . In this approach, they could deal with small-size systems, and the behavior of $z^{(q)}$ itself became unclear.

In order to improve this problem, we extend Resta's approach for Hermitian systems³⁰⁾ to the polarization in non-Hermitian systems, so that we rewrite Eq. (2) in terms of the right and left one-particle eigenstates:

$$z^{(q)} = \det S^{(q)},\tag{3}$$

$$S_{\mu,\nu}^{(q)}(k_{s},k_{s'}) = \sum_{j=1}^{L} \langle \psi_{k_{s}\mu}^{j,\mathrm{L}} | \mathrm{e}^{\mathrm{i}\frac{2q\pi}{L}x_{j}} | \psi_{k_{s'}\nu}^{j,\mathrm{R}} \rangle, \qquad (4)$$

where $k_s = (2\pi/L)(s + \theta/2\pi)$ with $s = 0, 1, \dots, L - 1$ for the

As such a fundamental relation, in this paper, we will point

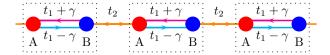


Fig. 1. (Color online) The non-Hermitian SSH model (9). The dotted boxes indicate the unit cells.

boundary conditions $|\psi_{k\mu}^{j+L,\alpha}\rangle = e^{i\theta} |\psi_{k\mu}^{j,\alpha}\rangle$, and the determinant is restricted to the occupied states. Then the determinant is rewritten as a product of the biorthogonal overlaps:

$$z^{(q)} = (-1)^{qN/L} \prod_{s=0}^{L-1} \prod_{\mu \in \text{occupied}} \langle u_{k_{s+q}\mu}^{L} | u_{k_{s}\mu}^{R} \rangle, \qquad (5)$$

where *N* is the number of electrons. The factor $(-1)^{qN/L}$ stems from the antisymmetry of the determinant.⁴⁰⁾ Since Eq. (5) is a simple product of overlaps between Bloch states with the wave vectors that differ by k_q , $z^{(q)}$ can be calculated for large system sizes, and the behavior of $z^{(q)}$ in the thermodynamic limit will be clarified.

We consider a two-band non-Hermitian system with chiral symmetry $\tau_3 H(k)\tau_3 = -H(k)$. In this case, the Hamiltonian is written as

$$H(k) = \begin{pmatrix} h_+(k) \\ h_-(k) \end{pmatrix}.$$
 (6)

Then we define the winding number as follows; $^{13-15)}$

$$\nu = \frac{\mathrm{i}}{2\pi} \int_0^{2\pi} \mathrm{d}k \, r^{-1}(k) \frac{\partial}{\partial k} r(k). \tag{7}$$

where $r(k) = h_+(k)/\sqrt{h_+(k)h_-(k)}$. For Hermitian systems, r^{-1} becomes r^* , and ν can only take 0 or 1. However, for non-Hermitian systems, the winding number ν can be half-integers.^{41–43}

For the two-band model with the single occupied band, the phase of the polarization is related to the winding number by Eq. (5) in the $L \rightarrow \infty$ limit as follows;

$$\ln z^{(1)} = i\pi + \sum_{s=0}^{L-1} \ln \langle u_{k_s}^{L} | u_{k_{s-1}}^{R} \rangle \simeq i(1 \pm \nu)\pi, \qquad (8)$$

which is well-defined unless v is half-odd integers, where the signs "±" are related to the choice of the eigenstates.¹⁵⁾

We concider the non-Hermitian Su-Schrieffer-Heeger (SSH) model with half-filling^{19,44,45)} as illustrated in Fig. 1. The Hamiltonian in real space is given by

$$\mathcal{H} = t_1 \sum_{i=1}^{L} c_{i,A}^{\dagger} c_{i,B} + t_2 \sum_{i=1}^{L} c_{i,B}^{\dagger} c_{i+1,A} + \text{H.c.}$$
$$+ \gamma \sum_{i=1}^{L} c_{i,A}^{\dagger} c_{i,B} - \text{H.c.}, \qquad (9)$$

where $c_{i,\alpha}$ ($c_{i,\alpha}^{\dagger}$) denotes the annihilation (creation) operator of a fermion in sublattice α at the *i*-th unit cell. When $\gamma = 0$, this model is Hermitian, and phase transitions occur at $t_1 = \pm t_2$. This Hamiltonian can be written as the quadratic form:

$$\mathcal{H} = \sum_{ij,\alpha\beta} c^{\dagger}_{i,\alpha} H_{ij,\alpha\beta} c_{j\beta}, \qquad (10)$$

so that it is diagonalized by the Fourier transformation $c_{k,\alpha}$ =

 $\sum_{j} \mathcal{U}_{kj} c_{j,\alpha}$ as follows:

$$\mathcal{H} = \sum_{k,\alpha\beta} c^{\dagger}_{k,\alpha} H_{\alpha\beta}(k) c_{k,\beta}, \qquad (11)$$

$$H(k) = \sum_{\mu=1}^{2} (d_{\mu} + if_{\mu})\tau_{\mu}, \qquad (12)$$

where

$$d_1 = t_1 + t_2 \cos k, \qquad f_1 = 0, d_2 = t_2 \sin k, \qquad f_2 = \gamma,$$
(13)

and τ_{μ} ($\mu = 1, 2, 3$) is Pauli matrices. This model has chiral symmetry, so that the energy eigenvalues are symmetric about zero energy. The square of the energy eigenvalue is given by

$$E^{2}(k) = t_{1}^{2} + t_{2}^{2} - \gamma^{2} + 2t_{1}t_{2}\cos k + i\,2t_{2}\gamma\sin k.$$
(14)

The energy gap closes at the exceptional points (EPs) $(d_1, d_2) = (-f_2, f_1)$ or $(f_2, -f_1)$, which leads to $t_1 = -t_2 \pm \gamma$ for k = 0 or $t_1 = t_2 \pm \gamma$ for $k = \pi$. For k = 0 and π , the energy eigenvalues are $E = \pm \sqrt{(t_1 + t_2)^2 - \gamma^2}$ and $\pm \sqrt{(t_1 - t_2)^2 - \gamma^2}$, respectively, so that they are pure imaginaries when t_1 satisfies $-t_2 - \gamma < t_1 < -t_2 + \gamma$ or $t_2 - \gamma < t_1 < t_2 + \gamma$, respectively [see Fig. 2(a)].

For the non-Hermitian SSH model in real space, we concider the "space inversion" as $\mathcal{P}c_{j,A(B)}\mathcal{P}^{-1} = c_{L+1-j,B(A)}$. Under this transformation, the non-Hermitian Bloch Hamiltonian (12) satisfies the following relation

$$\mathcal{P}H(k)\mathcal{P}^{-1} = H^{\dagger}(k), \qquad (15)$$

where $\mathcal{P} = \tau_1 \mathcal{K}$, and \mathcal{K} is a conjugate operator. Moreover, this transformation leads to

$$z^{(q)} = \langle \Psi_{\mathbf{R}} | \mathcal{P} U^q \mathcal{P}^{-1} | \Psi_{\mathbf{L}} \rangle = \mathrm{e}^{\mathrm{i}2q\pi N/L} [z^{(q)}]^{\dagger}.$$
(16)

Since N = L in the non-Hermitian SSH model at half-filling, we should choose q = 1. Then Eq. (5) is reduced to

$$z^{(1)} = (-1) \prod_{s=0}^{L-1} \langle u_{k_{s+1}-}^{L} | u_{k_{s}-}^{R} \rangle, \qquad (17)$$

where $|u_{k_{s-}}^{R(L)}\rangle$ is the right (left) eigenstate of the occupied band. For $t_2 + \gamma < t_1$, the electrons of the system are located on unit cells, so that we find that $z^{(1)} = -1$ for even *L* because $(2\pi/L) \sum_{x_{j=1}}^{L} x_j = \pi(L+1)$. Similarly, for $-t_2 + \gamma < t_1 < t_2 - \gamma$, the electrons of the system are located on between a unit cell and the neighboring one, so that we find that $z^{(1)} = 1$ for even *L* because of $(2\pi/L) \sum_{x_{j=1}}^{L} (2x_j + 1)/2 = \pi(L+2)$. On the other hand, for $-t_2 - \gamma < t_1 < -t_2 + \gamma$ or $t_2 - \gamma < t_1 < t_2 + \gamma$, the electrons of the system are located homogeneously, so that $z^{(1)} = 0$ for even *L* because $(2\pi/L) \sum_{x_{j=1}}^{L} (2x_j + 1/2)/2 = \pi(2L + 3)/2$. Here, we have used the fact that $z^{(1)}$ is always real, since Eq. (16) leads to $z^{(1)} = [z^{(1)}]^{\dagger}$ in the non-Hermitian SSH model.

The numerical results of the polarization $z^{(1)}$ for different system sizes are shown in Fig. 2(b), and $z^{(1)}$ distinguishes three topologically distinct phases $z^{(1)} = -1, 0, +1$, as expected. Here, we have used anti-periodic boundary conditions $c_{i+L,\alpha} = -c_{i,\alpha}$ to prevent divergences at EPs, at which phase transitions occur. The results do not depend on the boundary conditions except for the phase transition points. If the regions with Re E = 0 are interpreted as gapless phases, the

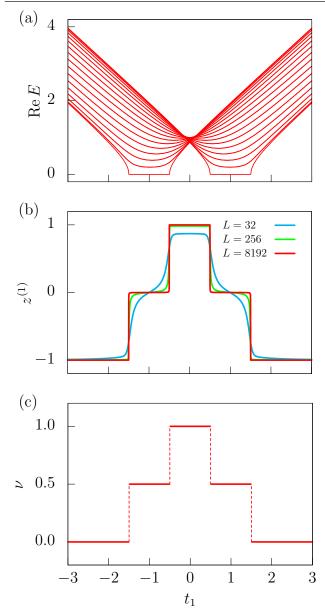


Fig. 2. (Color online) (a) The real part of energy eigenvalues, (b) the polarization and (c) the winding number in the non-Hermitian SSH model (9) with $t_2 = 1$ and $\gamma = 0.5$. The eigenvalues are computed for L = 32, and the polarization is calculated for L = 32, 256 and 8192.

results with $z^{(1)} = 0$ are consistent with the LSM theorem. Note that $z^{(1)}$ in a finite-size system has a finite value, so that $(2\pi)^{-1} \text{Im } \ln z^{(1)}$ is not a good quantity to determine topologically different phases, especially for $z^{(1)} = 0$ regions.

Using Eq. (7), we obtain the following winding number of the non-Hermitian SSH model:

$$\nu = \int_0^{2\pi} \frac{dk}{2\pi} \frac{t_2(t_1 \cos k + i\gamma \sin k + t_2)}{E^2},$$
 (18)

which is well defined except at EPs, where E^2 is given by Eq. (14). The winding number is equal to the half of the number of times that, in d_1 - d_2 plane, EPs are surrounded by the closed curve when k ranges from 0 to 2π .⁴¹

The numerical results of the winding number ν are shown in Fig. 2(c). Comparing them with the results of the polarization $z^{(1)}$ in the thermodynamic limit $(L \rightarrow \infty)$, we find that there are one-to-one correspondences between $\nu = 0, 1/2, 1$

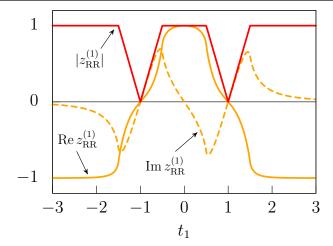


Fig. 3. (Color online) The real part (orange line), the imaginary part (orange dashed line) and the absolute value (red line) of the polarization, which is given by Eq. (19), in the non-Hermitian SSH model (9) with $t_2 = 1$ and $\gamma = 0.5$ for L = 8192.

and $z^{(1)} = -1, 0, +1$ for the topologically different phases. Therefore, Eq.(8) becomes singular at $z^{(1)} = 0$, and two quantities in this case can be well related as $z^{(1)} = -\cos \nu \pi$.

For comparison to the polarization $z^{(1)}$, we concider the polarization defined by the occupied right eigenstate. In the non-Hermitian SSH model, this is given by

$$z_{\rm RR}^{(1)} = (-1) \prod_{s=0}^{L-1} \langle u_{k_{s+1}-}^{\rm R} | u_{k_s-}^{\rm R} \rangle, \qquad (19)$$

where $|u_{k\mu}^{R}\rangle$ is normalized as $\langle u_{k\mu}^{R}|u_{k\mu}^{R}\rangle = 1$, and the numerical results are shown in Fig. 3. Unlike $z^{(1)}, z^{(1)}_{RR}$ is generally complex. We find that Re $z_{RR}^{(1)} \neq 0$ in the region that Re E = 0 and $\nu = 1/2$. Therefore, $z_{RR}^{(1)}$ is not a good index to characterize the different phases comparing with $z^{(1)}$. On the other hand, $|z_{RR}^{(1)}|$ shows liner behavior in terms of t_1 , and $|z_{RR}^{(1)}| \neq 1$ or $|z_{RR}^{(1)}| = 1$ correspond the phases with $\nu = 1/2$ and $\nu = 0, 1$, respectively. Thus $|z_{RR}^{(1)}|$ is better topological index than Re $z_{RR}^{(1)}$ and Im $z_{RR}^{(1)}$, in this case. Comparing the results of the twotypes of polarization *z* and z_{RR} defined by Eqs. (2) and (19), it is sufficient to use the former one given by a real number to describe the topological phases and transitions in the present non-Hermitian system as discussed in Ref. 6.

In wummary, we have studied an extension of the Resta's electronic polarization³⁰⁾ to non-Hermitian systems with chiral symmetry. We have given the reduction formalism for the polarization (5) which enables us to deals with large systems close to the thermodynamic limit. Then the relationship between the polarization and the winding number has been discussed.

We have analyzed the non-Hermitian SSH model and shown numerically that the polarization defined by the biorthogonal basis (2) takes three different values $z^{(1)} =$ -1, 0, +1 for the topologically distinct phases in the thermodynamic limit. We have also found that there is one-to-one correspondence with the winding number v = 0, 1/2, 1 defined in Refs. 17, 41. Furthermore, this relationship has been shown analytically as Eq. (8). Here we should be careful to take the thermodynamic limit of $z^{(1)}$: depending on how to take the thermodynamic limit, the region with v = 1/2 may be lost.⁴⁶⁾

The topological phases for the non-Hermitian skin effect in open systems have been discussed by a winding number in a different definition¹⁹⁾ from the present one for periodic systems. This winding number takes only two values, and the "transition point" where the winding number changes its value appears to be different. However their difference is only whether the integration is defined in the generalized Brillouin zone or in the ordinary Brillouin zone (7). Therefore the present study may contribute to analyze the skin effect by generalizing the polarization operator. There is another topological number "biorthogonal polarization" defined in open boundary systems.^{27,28)} This quantity is considered to characterize the number of edge modes.²⁸⁾ Therefore, despite having a similar appearance, there is no direct correspondence with the present electronic polarization.

We have also examined the polarization defined only by right eigenstates $z_{RR}^{(1)}$. This quantity takes a complex value and is not explicitly related to the winding number. In contrast to this, the polarization defined by the biorthogonal basis $z^{(1)}$ is a real number⁶⁾ and there is a clear one-to-one correspondence with the winding number, so that $z^{(1)}$ is considered to be more suitable definition than $z_{RR}^{(1)}$ for the present closed system.

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