Exact solution of single impurity problem in non-reciprocal lattices: impurity induced size-dependent non-Hermitian skin effect

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Non-Hermitian non-reciprocal systems are known to be extremely sensitive to boundary conditions, exhibiting diverse localizing behaviors and spectrum structures when translational invariance is locally broken, either by tuning the boundary coupling strength, or by introducing an effective boundary using impurities or defects. In this work, we consider the single impurity problem in the Hatano-Nelson model and the Su-Schrieffer-Heeger model, which can be exactly solved with the single impurity being treated as an effective boundary of the system. From our exact solutions for finite-size systems, we unveil that increasing the impurity strength can lead to a transition of the bulk states from non-skin to skin states, accompanied by the change of the spectrum structure from an ellipse in the complex plane to a segment along the real axis. These exact results indicate that the critical value of impurity strength is size-dependent, and increases exponentially with the lattice size when the impurity is strong or the system is large enough. Our exact solutions are also useful for determining the spectral topological transition in the concerned models.

I. INTRODUCTION

Boundary conditions play a pivotal role in determining the properties of a wide variety of physical systems, ranging from the most fundamental problem of solving a single-particle Schrödinger equation, to more stimulating emergent phenomena such as the quantum Hall effect, where the quantized Hall conductance is associated with the number of topological states localized at the physical boundaries of the system. In contrast, the bulk energy-spectra are usually expected to be insensitive to boundary perturbations, as their corresponding eigenstates are mostly distributed in the bulk of the system. However, this picture generally fails when non-Hermiticity is introduced to the Hamiltonian, where the spectra under periodic and open boundary conditions (PBC and OBC) can dramatically diverge from each other¹. Physically, such a significant boundary effect can be understood with the non-Hermitian skin effect (NHSE), namely a majority of eigenstates are pumped to the boundaries by the non-reciprocity of the system under OBC². To date, the NHSE has been extensively investigated in various systems,²⁻³⁵ as it is known to be associated with many intriguing non-Hermitian phenomena, e.g. the breakdown of conventional bulk boundary correspondence²,⁶, the spectral point-gap topology²⁹⁻⁻³¹, the critical NHSE³²,³³, and the directional signal amplification³⁴,³⁵.

Beyond the PBC and OBC, much effort has been made recently in exploring non-Hermitian systems with other types of boundary conditions. It has been found that by tuning the strength of boundary hoppings away from both the PBC and OBC, a new type of so-called scale-free accumulating states emerges in a finite-size system, and the NHSE becomes less stable against such boundary perturbations when increasing the system’s size³⁷,³⁸. The continuous deformation between the PBC and OBC also provides more insight of the NHSE²¹,³⁹, and leads to a topological quantized response unique in non-Hermitian systems⁴⁰. On the other hand, strong impurities and defects effectively induce a boundary in a periodic system, and may act as OBC for boundary phenomena in either Hermitian and non-Hermitian systems⁴¹⁻⁻⁴⁷.

In this paper, we analytically study the single impurity problem in two representative 1D non-Hermitian models that exhibit the NHSE under OBC, namely the Hatano-Nelson (HN) model and the non-reciprocal Su-Schrieffer-Heeger (SSH) model. In both cases, exact solutions are obtained with a single on-site impurity potential, whose strength varies from zero to infinity. The bulk states are seen to go through a transition from non-skin states to skin states at certain critical values of the impurity strength, after which their eigenenergies become purely real. In other words, a strong impurity behaves similarly as the OBC, except for the bound state localized at the impurity. The transition value of the impurity strength is found to depend on the system’s size and the non-reciprocity strength of the system, and also varies for different eigenstates. We have also applied our results to study the spectral topology of these two models, and the topological transition points are accurately predicted by our exact solutions.

The rest of the paper is organized as follows. In Sec. II, we present the exact solutions for the single-impurity problem in the HN model, and analyze in details the transition for the bulk states from non-skin to skin states. In Sec. III, we study the single-impurity problem for the non-reciprocal SSH model, where exact solutions can be obtained by mapping it to the HN model. We then applies our exact solutions to identify the topological transition points of the spectral topology of the two models.
The homogeneous equation can be solved by first solving its characteristic equation
\[ \epsilon = \frac{e^g}{z} + e^{-g} z. \]

Given an eigenenergy \( \epsilon \), there exist two solutions \( z_1 \) and \( z_2 \) satisfying the constraint condition
\[ z_1 z_2 = e^{2g}, \]
and thus the eigenenergies can be represented as \( \epsilon = (z_1 + z_2) e^{-g} \). The general wavefunction takes the form of
\[ \psi_n = \alpha_1 z_1^n + \alpha_2 z_2^n, \]
which fulfills the bulk eigen-equation of Eq. (2). To obtain the eigensolutions of the whole system, the general ansatz of wave function in Eq.(7) shall also satisfy the boundary conditions. Substituting Eq.(7) into Eq.(3) and Eq.(4), we obtain
\[ M_B \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} A(z_1, N) & A(z_2, N) \\ B(z_1, N) & B(z_2, N) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = 0 \]
with
\[ A(z, N) = e^{-g} z + e^g z^{-1} - \epsilon + V_0 \]
and
\[ B(z, N) = e^g z^{-2} + e^{-g} - \epsilon z^{-1}. \]

The existence of nontrivial solutions for \((\alpha_1, \alpha_2)\) is determined by \( \det[M_B] = 0 \), which gives rise to the general solution with \( \alpha_1 \neq 0, \alpha_2 \neq 0 \):
\[ (z_1^{N+1} - z_2^{N+1}) - \frac{t_R}{t_L} (z_1^{N-1} - z_2^{N-1}) - \left[ 1 + \left( \frac{t_R}{t_L} \right)^N \right] (z_1 - z_2) - \frac{V_0}{t_L} (z_1^{N} - z_2^{N}) = 0. \]

Eq.(9) and Eq.(6) together determine the solution of \( z_1 \) and \( z_2 \) exactly. Following the constraint condition of Eq.(6), we can always rewrite the solutions as
\[ z_1 = r e^{i\theta}, \quad z_2 = r e^{-i\theta} \]
with \( r = \sqrt{\frac{V_0 t_L}{t_R}} = e^{g} \). Note that \( \theta \) is not restricted to be real, which is important in determining the properties of the spectrum in latter discussion. Thus Eq.(9) becomes
\[ 2 \cos[N\theta] \sin \theta - (r^{-N} + r^{N}) \sin \theta - V_0 \sin[N\theta] = 0, \]
or equivalently
\[ \frac{\sin \theta [2 \cos(N\theta) - 2 \cosh(Ng)]}{\sin(N\theta)} = V_0. \]

Defining \( e^{i\theta} \equiv \beta \), Eq. (11) becomes a polynomial equation of \( \beta \) with an order of \( 2N \), and hence shall have
the coefficients to the same eigenenergies, and the same eigenstates as $|\theta_{k,i}| = g = 1$. The gray dotted line (vertical) represents $V_0 = 2 \sinh(gN) = 1.2 \times 10^6$ for the chosen parameters. (b) The corresponding complex spectra of bulk states for the system with $V_0 = 10^2$, $7 \times 10^3$, and $2 \times 10^6$, respectively.

Further analysis in appendix A, we find that $\theta_k$ is always real when $V_0$ exceeds a critical value $V_{0,c}$, with

$$V_{0,c} \approx 2 \sinh(Ng) \approx e^{Ng}$$

when $N \geq 1$. For relatively small $N$, the actual critical value $V_{0,c}$ is slightly smaller than $2 \sinh(Ng)$. Fig. 2(a) shows the imaginary part $\theta_{k,i}$ for the system with $g = 1$ and $N = 14$ as a function of $V_0$, with $V_0 = 2 \sinh(Ng)$ given by the gray dotted line. When $0 < V_0 \lesssim 8.6 \times 10^4$, we obtain $|\theta_{k,i}| > 0$ for every $k$, and the spectrum still forms an ellipse, as shown in the top panel of Fig. 2(b). We note that the bound state is omitted and the eigenenergies of bulk states are demonstrated in Fig. 2(b). For $8.6 \times 10^4 \lesssim V_0 < 2 \sinh(Ng)$, $\theta_{k,i}$ becomes zero for some values of $k$, meaning that a part of the spectrum becomes real, as shown in the middle panel of Fig. 2(b). Due to the pseudo-Hermiticity, the non-real eigenenergies in the above two cases always come in pairs with complex conjugated values of $\theta$, and hence the same $|\theta_{k,i}|$. When $V_0 \geq 2 \sinh(Ng)$, all $\theta_{k,i} = 0$ for bulk states, i.e. all $\theta_k$ and eigenenergies are real, as shown in the bottom panel of Fig. 2(b).

Next we consider the behaviors of the eigenstates. When $V_0 > 0$, the eigenstates (7) can be written as

$$\psi_{n}^{k} = e^{ng}(\alpha_1 e^{-i\theta_k} + \alpha_2 e^{-i\theta_k})$$

which are uniformly distributed. Notes that in this case $A(z_1, N) = 0$, allowing us to omit the branch $z_2$.

We then move on to the more sophisticated case where $V_0 \neq 0$. We first rewrite $\theta_k$ as $\theta_k = \theta_{k,r} + i\theta_{k,i}$, where $\theta_{k,r}$ and $\theta_{k,i}$ are the real and imaginary part of $\theta_k$. The energy $\epsilon_k$ is real either when $\theta_{k,i} = 0$ or $\theta_{k,r} = (\pi/2)/2$, otherwise it acquires a nonzero imaginary amplitude. With
\( \alpha_2/\alpha_1 \gg 1 \) and \( \psi_n^k \propto e^{n(x-|\theta_{k,i}|)}e^{i \theta_{k,i}} \) when \( \theta_{k,i} < 0 \). Similar results can also be obtained for \( g < 0 \). Overall, the wavefunction can be written as
\[
\psi_n^k \approx \alpha e^{\delta |g|(|g|-|\theta_{k,i}|)}e^{i \theta_{k,i}},
\]
with \( \alpha = \max(\alpha_1, \alpha_2) \), and the wavefunction decays with increasing \( n \) when \( |\theta_{k,i}| > |g| \), and with decreasing \( n \) when \( |\theta_{k,i}| < |g| \). In Fig. 2(a), it is seen that \( |\theta_{k,i}| > |g| \) is satisfied only in a regime with small \( V_0 \). Therefore we zoom in and provide a clearer view of this regime in Fig. 3(a). When \( V_0 \lesssim 4.5 \), some \( \theta_{k,i} \) are seen to be greater than \( |g| = 1 \), and the corresponding eigenstate \( \psi_n^k \) decays to the right, as shown in Fig. 3(b1). When \( V_0 \geq 4.5 \), all \( \theta_{k,i} \) satisfy \( |\theta_{k,i}| < g \), and the corresponding \( \psi_n^k \) decays to the left, as shown in Fig. 3(b2).

When \( V_0 \geq 2 \sinh(n \alpha g) \), \( \theta_{k,i} = 0 \) is obtained for all bulk states, and the wavefunction \( \psi_n^k \propto e^{g n \alpha e^{i \theta_{k,i}}} \) takes the form of skin states. That is, all bulk states now become skin states and all the eigenenergies are real, which is the same situation as the system with \( V_0 = 0 \) but under OBC. To see clearly the transition from the non-skin states to skin states, we calculate the averaged inverse participation ratio (IPR) to characterize the localization of the system,
\[
\langle \text{IPR} \rangle = \frac{1}{N} \sum_k \frac{\sum_n |\langle n | \psi^k \rangle|^4}{\langle \psi^k \psi^k \rangle^2},
\]
where \( |\psi^k \rangle \) is the \( k \)-th right eigenstate of Hamiltonian (1). The non-skin states given by Eq. (15) are sensitive to \( V_0 \) and size \( N \), suggesting that variation of \( V_0 \) or \( N \) can change (IPR) significantly, analogous to the scale-free accumulating states in Ref. [37]. On the other hand, the locality of skin states only depends on \( g \) and shall give a constant \( \langle \text{IPR} \rangle \) independent from the impurity strength \( V_0 \). We display the (IPR) for all bulk states versus \( V_0 \) in Fig. 4, which indicates a clear transition from non-skin to skin states at \( V_0 = 2 \cosh(n \alpha g) \). That is, as \( V_0 \) is increased, (IPR) increases before the transition point of \( V_0 = V_{0,c} \), and remains a constant for the skin states after the transition.

![FIG. 4: Average IPR for the system (1) with \( N = 14 \), \( g = 0.2 \), 0.5, and 1, respectively. The dashed lines represent the transition points from non-skin to skin states: \( V_0 = 2 \cosh(Ng) \).](image)

![FIG. 5: Spectrum \( |E| \) for the system (16) with \( N = 20 \), \( g = 1 \), (a) \( V = 2 \cosh(4) \) and (b) \( V = 2 \cosh(N + 1) \), respectively. The dashed lines in (a) represent the gap-closing points \( t' = \pm e^{\pm g} \). The dashed lines in (b) represent the gap-closing points \( t' = \pm 1 \).](image)

in the momentum space, where \( h_x = t' \cos k + \cosh g \), \( h_y = t' \sin k - i \sin g \) with \( 0 \leq k < 2\pi \), and \( \sigma_x, \sigma_y \) are the Pauli matrices. The eigenenergies are given by
\[
E = \pm \sqrt{(h_x + ih_y)(h_x - ih_y)}
= \pm \sqrt{(t'e^{ik} + e^g)(t'e^{-ik} - e^{-g})}.
\]

III. SINGLE IMPURITY IN NON-RECIPROCAL SSH MODEL

The non-reciprocal SSH model with a single impurity under PBC, as displayed in Fig. 1(b), can also be exactly solved. The Hamiltonian is given by
\[
H_{SSH} = \sum_{n=0}^{N-1} \left[ (t e^{-g} |n, A\rangle \langle n, B| + e^g |n, B\rangle \langle n, A|) + \right. \\
+ t' (|n, B\rangle \langle n + 1, A| + h.c.) + V_0 |0, A\rangle \langle 0, A|,
\]
with A and B indexes for different sublattices, \( |N, A(B)\rangle \equiv |0, A(B)\rangle \), \( N \) the total number of unit cells, \( V_0 \) the impurity strength, and \( t' (te^{\pm g}) \) the inter-cell (right and left intra-cell) hopping term(s). The energy unit is set to be \( t = 1 \) for latter convenience.

When \( V_0 = 0 \), through the Fourier transformation, the Hamiltonian of the non-reciprocal SSH model without the impurity can be represented as
\[
H_0 (k) = h_x \sigma_x + h_y \sigma_y
\]
The two-band structure of this model allows line-gap topology to emerge in this system, and the phase boundaries can be determined by the gap closing conditions of the system,\(^2,3\),

\[ t' = -e^{\pm g} \quad \text{and} \quad t' = e^{\pm g}. \]  

(17)

Note that through the similarity transformation, the model \((16)\) with \(V_0 = 0\) under OBC becomes the Hermitian SSH model, where the topological transition points (gap-closing points) are given by \(t' = \pm t = \pm 1\). In other words, the spectra of systems under PBC and OBC have different gap-closing points.\(^2,6,38\)

When \(V_0 \neq 0\), we can solve Eq. \((16)\) by taking the wavefunction as \(\psi = \sum_n (\psi_{A,n} |n, A\rangle + \psi_{B,n} |n, B\rangle)\). The stationary Schrödinger equation \(H_{SSH} |\psi\rangle = E |\psi\rangle\) is equivalent to the following difference equations

\[ e^g \psi_{A,n-1} + t' \psi_{A,n} = E \psi_{B,n-1}, \]  

(18)

\[ t' \psi_{B,n-1} + e^{-g} \psi_{B,n} + \delta_{x,0} V_0 \psi_{A,n} = E \psi_{A,n}, \]  

(19)

where \(E\) is the eigenenergy, Eq.\((18)\) gives us

\[ \psi_{B,n} = \frac{e^g}{E} \psi_{A,n} + \frac{t'}{E} \psi_{A,n+1}. \]  

(20)

We can decouple \(\psi_A\) and \(\psi_B\) by substituting Eq.\((20)\) into Eq.\((19)\), which yields

\[ e^g \psi_{A,n-1} + e^{-g} \psi_{A,n+1} + \delta_{x,0} \frac{EV_0}{t'} \psi_{A,n} = \frac{E^2 - t'^2 - 1}{t'} \psi_{A,n}. \]  

(21)

It is obvious that Eq. \((21)\) under the following substitution

\[ V_0 \rightarrow \frac{EV_0}{t'}, \]  

(22)

\[ \epsilon \rightarrow \frac{E^2 - t'^2 - 1}{t'}. \]  

(23)

is identical to Eq. \((2)\) with boundary conditions \((3)\) and \((4)\). Thus to solve Eq. \((21)\), we can directly use the results of the impurity problem in the HN model in section II. That is, by substituting Eqs. \((23)\) and \((22)\) into Eqs. \((13)\) and \((12)\), we obtain

\[ E = \pm \sqrt{1 + t'^2 + 2t' \cos \theta} \]

and

\[ \frac{t' \sin(\theta) (2 \cos(N \theta) - 2 \cosh(N g))}{\pm \sqrt{1 + t'^2 + 2t' \cos \theta \sin(N \theta)}} = V_0 \]  

(24)

respectively. Following our analysis of Eq. \((12)\), the transition point from non-skin states to skin states can be determined by

\[ V_{0,c} = 2t^* \sinh(N g) \approx t^* e^{Ng} \]

with \(t^* = \min\{1, t'\} \) for large \(N \) or \(g \). \(V_{0,c}\) increases exponentially with the lattice size \(N \). At small \(V_{0,c}\), it is far from the critical value, all \(\theta_k\) for bulk states are complex. The spectra are similar to the system with \(V_0 = 0\). The topological phase transition occurs at \(t' = \pm e^{\pm g} \), as shown in Fig. \(5\) \(a\). When \(V_0 \geq 2t^* \sinh(N g)\), all \(\theta_k\) for bulk states are real. So all the bulk states become the skin states and all the eigenenergies are real, analogous to the system with \(V_0 = 0\) under OBC. The topological phase transition then takes place at \(t' = \pm 1\), as shown in Fig. \(5\) \(b\).

Finally, we display (IPR) of all bulk states versus \(V_0\) in Fig. \(6\) with \(t' = 0.5\) and \(t' = 2\), respectively. Fig. \(6\) demonstrates a clear transition from non-skin states to skin states at \(V_0 = \sinh(N g)\) with \(t' = 0.5\) and \(V_0 = 2 \sinh(N g)\) with \(t' = 2\) for \(N = 14\). (IPR) increase for the non-skin states with increasing \(V_0\), and remains constant for the skin states.

IV. QUANTIZED RESPONSE OF THE SPECTRAL TOPOLOGY IN THE IMPURITY MODELS

In previous sections, we have exactly solved the single-impurity problem for the HN model and SSH model, both exhibit the NHSE and thus possess a non-trivial spectral topology.\(^{29–31}\) It has recently been discovered that a quantized response corresponding to the spectral topology can be extracted from the system’s Green’s function element, in the process of tuning the boundary condition from PBC to OBC continuously.\(^{40}\) Therefore we expect a similar phenomenon to arise also in our model, as a strong impurity strength effectively acts as the OBC.
Following Ref. [40], we define quantities as
\[ \nu_0(N-1) = \frac{\partial \ln G_0(N-1)}{\partial \ln V_0}, \quad \nu^B_0(N-1) = \frac{\partial \ln G^B_0(N-1)}{\partial \ln V_0} \] (25)
for the HN model and the SSH model respectively, with
\[ G_0(N-1) = \langle 0 | G_{\text{HN}} | N - 1 \rangle \]
and
\[ G^B_0(N-1) = \langle 0, B | G_{\text{SSH}} | N - 1, B \rangle \]
the off-diagonal elements of the Green's functions \( G_{\text{HN}} \) of the HN model and \( G_{\text{SSH}} \) of the SSH model,
\[ G_{\text{HN}} = (E_r - H_{\text{HN}})^{-1}, \quad G_{\text{SSH}} = (E_r - H_{\text{SSH}})^{-1}. \] (26)

\( E_r \) is a chosen complex reference energy to define the spectral winding \cite{30,31,40}. In our models, the spectral winding number is \( \nu = 1 \) for \( E_r \) enclosed by the PBC spectra in the complex plane. In such cases, \( \nu_0(N-1) \) and \( \nu^B_0(N-1) \) are expected to jump from 1 to 0 for the concerned models when \( V_0 \) is increased and reaches a critical value, where the spectra coincide with \( E_r \) \cite{40}.

In Fig. 7, we illustrate the defined quantities as functions of \( V_0 \) for several different \( E_r \) enclosed by the PBC spectrum at \( V_0 = 0 \). It is seen that each of \( \nu_0(N-1) \) and \( \nu^B_0(N-1) \) roughly exhibits a plateau at 1, and jumps to 0 after a critical value \( V_0 = V_c \). Note that \( V_c \) is distinguished from \( V_{0,c} \) in previous sections, which describes the transition to a fully real spectrum. The spectrum forms a shrinking ellipse with increasing \( V_0 \), passing through \( E_r \) at \( V_0 = V_c \), after which the spectral winding jumps from 1 to 0. Therefore for a given \( E_r \), we can require it to be an eigenenergy \( \epsilon \) of the system, then determine \( V_c \) through Eqs. (12) and (24) for the two models respectively.

We would also like to point out that in a finite-size system, the spectral flow [cyan dotted curves in Fig. 7(a) and (b)] from \( V_0 = 0 \) to \( V_0 \to \infty \) cannot cover the regime enclosed by the PBC ellipse-spectrum completely. Strictly speaking, a real \( V_c \) can be obtained only when \( E_r \) exactly falls along the spectral flow. Nevertheless, numerically we can choose \( E_r \) close enough to the spectral flow [blue and red stars in Fig. 7(a) and (b)], and the absolute value of the obtained \( V_c \) are seen to be in good consistency with the jump of \( \nu_0(N-1) \) and \( \nu^B_0(N-1) \) in Fig. 7(c) and (d) respectively.

V. SUMMARY

In summary, we have exactly solved the impurity problem in the HN model and the SSH model. The exact solutions of finite-size systems reveal a transition for the bulk states from non-skim states to skin states when increasing the impurity strength \( V_0 \), and the corresponding complex eigenenergies also become real after the transition. The critical value \( V_{0,c} \) of the impurity for the transition depends on both the lattice size \( N \) and the parameter \( g \) describing the non-reciprocity, and increases as \( V_{0,c} = \sinh N g \), \( \sinh N g \) serves as exact \( V_{0,c} \) in the large \( N \), while still of high accuracy in the small \( N \), despite the value of \( g \). Such a transition indicates that a strong impurity acts as an open boundary for the NHSE in non-reciprocal non-Hermitian systems. Different bulk states are also found to reach the OBC limit at different critical values of \( V_{0,c} \). We have also extended our study to the single-impurity problem of the SSH model, which can be mapped to the HN model, and exact solutions can be obtained accordingly. Our exact solutions are also proven useful for investigating the spectral topological transition in the concerned models.

\[ \text{Acknowledgments} \]

The work is supported by NSFC under Grants No.11974413 and the National Key Research and Development Program of China (2016YFA0300600 and 2016YFA0302104). L. L. acknowledges funding support by the Guangdong Basic and Applied Basic Research Foundation (No. 2020A1515110773).
FIG. 8: $f_1(\theta)$ and $f_2(\theta)$ with $V_0 = 2\sinh[Ng]$ as function of $\theta$. Parameters given in (a) $N = 14, g = 1$; (b) $N = 14, g = 0.1$; (c) $N = 4, g = 1$; (d) $N = 4, g = 0.1$; (e) $N = 7, g = 1$; and (f) $N = 7, g = 0.1$. Dash lines separate different period of $f_1(\theta)$.

Appendix A: The transition point between complex and real spectra

From Fig. 2 we see that the spectrum of the HN model with an impurity becomes purely real when $V_0$ is large enough. To identify the critical value $V_c$ for this transition, we rewrite Eq. (11) as

$$f_1(\theta) = f_2(\theta), \quad (A1)$$

where

$$f_1(\theta) = \frac{2 \cos[N\theta] - (r^{-N} + r^N)}{\sin[N\theta]} = \frac{2 \cos[N\theta] - 2 \cosh(Ng)}{\sin[N\theta]}, \quad (A2)$$

and

$$f_2(\theta) = \frac{V_0}{\sin\theta}. \quad (A3)$$

Note that the energy

$$\epsilon = 2 \cos \theta$$

is real with either purely real or imaginary $\theta$. We shall first focus on the case with real $\theta$, which has a period of $2\pi$. On the other hand, $\theta$ and $-\theta$ correspond to the same eigensolution of the system, as discussed in the main text. Therefore we only need to focus on the behavior of $f_{1,2}(\theta)$ with $\theta \in (0, \pi)$. Here the two points of $\theta = 0$ and $\pi$ are excluded, because at such values we shall obtain a non-physical solution with a vanishing wavefunction $\phi_n = 0$ by substituting Eq. (10) into Eq. (8) in the main text. If $f_1(\theta)$ and $f_2(\theta)$ have $N-x$ intersection points, Eq. (A1) has $N-x$ real and $x$ complex solutions, where $0 \leq x < N$. In this regime, $f_2(\theta)$ is a positive definite function, which is symmetrical of $\theta = \pi/2$ and its minimum value is given by $f_{2,\text{min}} = f_2(\pi/2) = V_0$. $f_1(\theta)$ has a period of $2\pi/N$ (separated by the dash lines in Fig. 8), and satisfies $f_1(\theta) > 0$ in the regime of

$$\theta \in \left(\frac{(2n+1)\pi}{N}, \frac{(2n+2)\pi}{N}\right), \quad n = 0, 1, \ldots, \left\lfloor \frac{N}{2} \right\rfloor - 1,$$

i.e. the right half of each period. In each interval, $f_1(\theta)$ decreases monotonically at first and meets its minimum value $f_{1,\text{min}} = 2\sinh(Ng)$ at

$$\theta = \frac{1}{N}(\arccos \frac{1}{\cosh(Ng)} + 2n\pi), \quad n = 1, \ldots, [N/2],$$

and increases monotonically again (see Fig. 8). Therefore $f_1(\theta)$ and $f_2(\theta)$ generally intersect twice within each of the $[N/2]$ intervals given by Eq. (A4). However, for an even $N$, the second intersection in the last interval tends to $\theta = \pi$ where both $f_1(\theta)$ and $f_2(\theta)$ tend to infinity. Thus we obtain $N-1$ intersections of $f_1(\theta)$ and $f_2(\theta)$ in total for $\theta \in (0, \pi)$, with either an even [Fig. 8(a)-(d)] or an odd $N$ [Fig. 8(e) and (f)]. When $N \to \infty$, the period of $f_1(\theta)$ approaches zero, meaning we can find the minimum value of $f_1(\theta)$ infinitely close to $\pi/2$, leading to

$$\lim_{N \to \infty} V_{0,c} = 2\sinh(Ng),$$

and two intersections around this nadir emerge when $V_{0,c} > 2\sinh(Ng)$. As we can infer from Fig. 8(c) and (d), $2\sinh(Ng)$ makes a good approximation of $V_{0,c}$ also for small $N$. The exact critical value of $V_{0,c}$ can only be smaller than $2\sinh(Ng)$, as $f_2(\theta)$ gets larger when $\theta$ diverges away from $\pi/2$, and hence approaches the minimums of $f_1(\theta)$ at a smaller $V_0$. To conclude, when $V_0 \geq 2\sinh(Ng)$, $f_2(\theta)$ and $f_1(\theta)$ shall have $N-1$ intersections for $\theta \in (0, \pi)$, corresponding to $N-1$ real solutions of the bulk states.

For imaginary $\theta$, $f_1(\theta)$ and $f_2(\theta)$ are mostly monotonic and only gives a single intersection for $\Im[\theta] \in (0, \infty)$, regardless of the value of $N$ and $g$, corresponding to the bound state.
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