Exact solution to the Su-Schrieffer-Heeger model with open boundaries

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We present an exact solution to the Su-Schrieffer-Heeger model with open boundaries[*1]. The Hamiltonian is given by

$$\hat{H} = v \sum_{n=1}^{L} \left(\hat{b}_n^\dagger \hat{a}_n + \hat{a}_n^\dagger \hat{b}_n \right) + t \sum_{n=1}^{L} \left(\hat{a}_{n+1}^\dagger \hat{b}_n + \hat{b}_n^\dagger \hat{a}_{n+1} \right), \tag{1}$$

where $\hat{a}_n$ and $\hat{b}_n$ ($\hat{a}_n^\dagger$ and $\hat{b}_n^\dagger$) represent the fermion annihilation (creation) operators on the two sublattices. For simplicity, we assume that the hopping amplitudes are positive, i.e., $v, t > 0$.

Let $E \in \mathbb{R}$ be a single-particle eigenenergy and $\hat{\varphi} = \sum_{n=1}^{L} (A_n \hat{a}_n + B_n \hat{b}_n)$ be the corresponding single-particle eigenstate with coefficients $A_n, B_n \in \mathbb{C}$. The Schrödinger equation $[\hat{H}, \hat{\varphi}] = E \hat{\varphi}$ reads

$$\begin{aligned} tB_{n-1} + vB_n &= EA_n \quad (n = 2, 3, \cdots, L), \\ vA_n + tA_{n+1} &= EB_n \quad (n = 1, 2, \cdots, L-1) \end{aligned} \tag{2}$$

in the bulk, and

$$vB_1 = EA_1, \quad vA_L = EB_L \tag{3}$$

at the edges. By defining A_{L+1} and B_0 through Eq. (2), the boundary conditions (3) reduce to

$$A_{L+1} = B_0 = 0. \tag{4}$$

Now, we take a plane-wave ansatz $A_n \sim A e^{\mathrm{i}kn}, B_n \sim B e^{\mathrm{i}kn}$ ($k \in \mathbb{C}$). While the wave number is real ($k \in \mathbb{R}$) for delocalized states, it is no longer real for localized states. The bulk equation (2) reduces to

$$\begin{pmatrix} 0 & v + te^{-\mathrm{i}k} \\ v + te^{\mathrm{i}k} & 0 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = E \begin{pmatrix} A \\ B \end{pmatrix}. \tag{5}$$

For a nontrivial solution, we have the energy dispersion relation

$$E(k) = \pm \sqrt{v^2 + t^2 + 2vt \cos k}. \tag{6}$$

If an eigenstate with wave number $k \in \mathbb{R}$ belongs to an eigenenergy $E \in \mathbb{R}$, another eigenstate with wave number $-k$ belongs to the same eigenenergy E. Thus, a generic eigenstate is described by

$$A_n = A_+ e^{\mathrm{i}kn} + A_- e^{-\mathrm{i}kn}, \quad B_n = B_+ e^{\mathrm{i}kn} + B_- e^{-\mathrm{i}kn} \tag{7}$$

[*1] I learned this technique from Hosho Katsura during my fourth year as an undergraduate student in his group and wrote a paper [K. Kawabata, R. Kobayashi, N. Wu, and H. Katsura, *Exact zero modes in twisted Kitaev chains*, Phys. Rev. B **95**, 195140 (2017) [arXiv:1702.00197]. It was also helpful for my subsequent research on topological phases of non-Hermitian systems; see, for example, Appendix I of Phys. Rev. X **9**, 041015 (2019) [arXiv:1812.09133].

with $A_+, A_-, B_+, B_- \in \mathbb{C}$. From the bulk eigenequation (5), we obtain

$$\frac{B_+}{A_+} = \frac{v + te^{\mathrm{i}k}}{E(k)} =: C(k)\,, \tag{8}$$

and similarly, $B_-/A_- = C(-k)$.

The boundary equation (4) leads to the quantization of the wave number k. Specifically, Eq. (4) leads to

$$\begin{pmatrix} e^{\mathrm{i}k(L+1)} & e^{-\mathrm{i}k(L+1)} \\ C(k) & C(-k) \end{pmatrix} \begin{pmatrix} A_+ \\ A_- \end{pmatrix} = 0, \tag{9}$$

which has a nontrivial solution if and only if the determinant of the coefficient matrix vanishes. After some calculations **(please check)**, we obtain the quantization condition

$$\frac{\sin k(L+1)}{\sin kL} = -\frac{t}{v} \tag{10}$$

which determines the possible values of k (see Fig. 1 for the behavior of the left-hand side of this equation). In the trivial phase ($t < v$), all the wave numbers k are real, and thus all the corresponding eigenstates are delocalized throughout the system. In the topological phase ($t > v$), on the other hand, some of the wave numbers k are no longer real, and the concomitant eigenstates are localized at the edges.

To determine the localization length, we set $k = \pi + \mathrm{i}q$ ($q \in \mathbb{R}$), yielding

$$\frac{t}{v} = \frac{\sinh q(L+1)}{\sinh qL} \to e^{|q|} \quad (L \to \infty)\,. \tag{11}$$

Notably, the eigenstates behave like $\sim (-1)^n e^{qn}$, and hence the localization length is given as $1/|q| \simeq 1/\log(t/v)$. From the energy dispersion in Eq. (6), the corresponding eigenenergies are obtained as

$$E = \pm\sqrt{v^2 + t^2 + 2vt\cos(\pi + \mathrm{i}q)} = \sqrt{v^2 + t^2 - vt\left(e^q + e^{-q}\right)} \to 0 \quad (L \to \infty)\,. \tag{12}$$

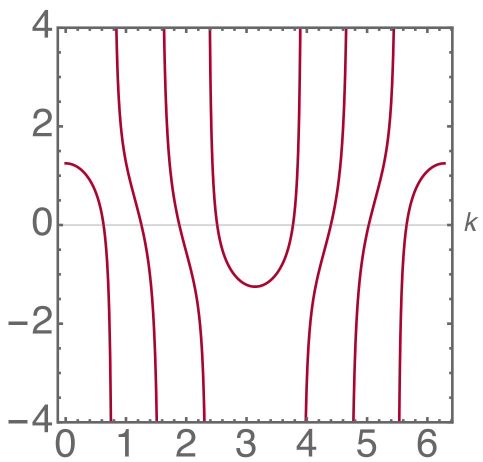

Fig. 1: Left-hand side of the quantization condition in Eq. (10) [i.e., $\sin k(L+1)/\sin kL$] for $L = 4$.