

# Memo: Wannier States and Spectral Flow

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This is a memo explaining that, in an insulator, if exponentially localized Wannier states can be constructed for both the occupied and unoccupied states, then no spectral flow exists for any real-space boundary, including boundaries of higher-order insulators. This is equivalent to the statement in Sec. II-A of Ref. [1].

Let  $H_{\mathbf{k}}$  be a Hamiltonian with  $N$  degrees of freedom per unit cell; thus  $H_{\mathbf{k}}$  is an  $N \times N$  matrix. Denote the degrees of freedom inside a unit cell by  $|\mathbf{x}\alpha\rangle$ . The Hamiltonian is

$$H = \sum_{\alpha\beta, \mathbf{x}\mathbf{x}'} h_{\alpha,\beta}(\mathbf{x} - \mathbf{x}') |\mathbf{x}\alpha\rangle \langle \mathbf{x}'\beta|. \quad (1)$$

Assume that  $h_{\alpha\beta}(\mathbf{x})$  decays exponentially, and assume a spectral gap. Suppose that, for both the occupied and unoccupied states, one can construct exponentially localized Wannier states  $w_{n\mathbf{R}}$  preserving the symmetry. Here ‘‘preserving the symmetry’’ means that a symmetry operation maps a Wannier state  $w_{n\mathbf{R}}$  to a linear combination of Wannier states  $w_{n'\mathbf{R}'}$  at the transformed site  $\mathbf{R}'$ .

Since the degrees of freedom defining  $H_{\mathbf{k}}$  can be expanded in the Wannier basis, the Hamiltonian becomes a short-range hopping model in that basis:

$$H = \sum_{nn', \mathbf{R}\mathbf{R}'} t_{nn'}(\mathbf{R} - \mathbf{R}') |Rn\rangle \langle R'n'|. \quad (2)$$

Here  $t_{nn'}(\mathbf{R} - \mathbf{R}')$  decays exponentially. If exponentially localized Wannier states do not exist, then  $t_{nn'}(\mathbf{R} - \mathbf{R}')$  becomes long-ranged.

Now flatten  $H$  while preserving the gap and the symmetries. Denote the flattened Hamiltonian by  $H'$ . In the Wannier basis,  $H'$  is an atomic insulator:

$$H' = \sum_{n\mathbf{R}} \epsilon_{n\mathbf{R}} |Rn\rangle \langle Rn|. \quad (3)$$

Notice that the interpolation

$$H_t = (1 - t)H + tH', \quad t \in [0, 1], \quad (4)$$

preserves the presence or absence of spectral flow. As a boundary condition, consider OBC for the Wannier basis  $|Rn\rangle$ :

$$\phi_n(\mathbf{R}) = 0, \quad R_x > 0. \quad (5)$$

Then the spectrum is exactly given by  $\epsilon_{n\mathbf{R}}$ . Alternatively, if degrees of freedom also exist for  $R_x > 0$ , they become zero states. Equation (5) is also some boundary condition in the original basis  $|\mathbf{x}\alpha\rangle$ . If one assumes that the presence or absence of spectral flow does not depend on the boundary condition, then the existence of exponentially localized Wannier states for both occupied and unoccupied states proves the absence of spectral flow.

Remark: in general, a boundary condition may also be specified by a boundary Hamiltonian  $H_{\text{bdy}}$  near the boundary. Let the OBC in the original basis be denoted by  $H_{\text{bdy}}$ , and the OBC (5) in the Wannier basis by  $H_{\text{W,bdy}}$ . One can ask whether spectral flow appears under the continuous change of boundary condition

$$(1 - s)H_{\text{W,bdy}} + sH_{\text{bdy}}. \quad (6)$$

As long as the gap remains open, spectral flow is invariant under continuous deformation, so its presence or absence does not change.

Memo:

- A realistic Hamiltonian has infinitely many unoccupied states. How should this case be treated?

## References

- [1] Alexander Altland, Piet W. Brouwer, Johannes Dieplinger, Matthew S. Foster, Mateo Moreno-Gonzalez, and Luka Trifunovic, *Fragility of Surface States in Non-Wigner-Dyson Topological Insulators*, Phys. Rev. X 14, 011057, published 27 March 2024.