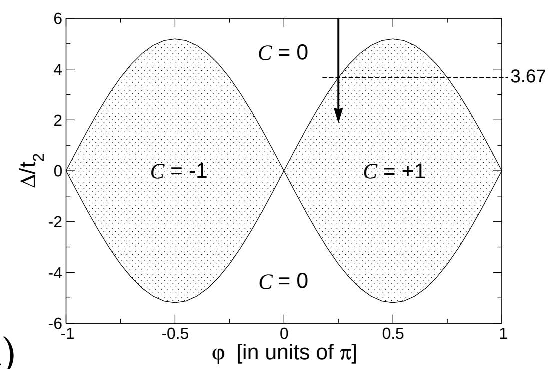
On the Impossibility of Constructing Maximally Localized Wannier Functions in Chern Insulators

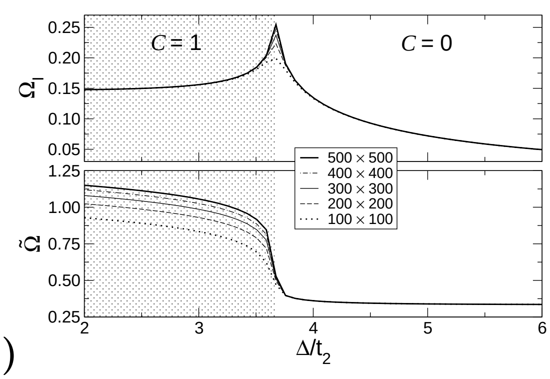
Timo Thonhauser[1,2] and David Vanderbilt[1]

[1] *Department of Physics and Astronomy, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA.*
[2] *Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA.*

The Haldane model [1] is a simple tight-binding model that exhibits a regular insulating phase ($C = 0$) as well as a Chern-insulator phase ($C = \pm 1$), depending on the model parameters φ and Δ/t_2 (see Fig. a). This provides us with a simple means to study the behavior of several physical properties as the system turns into a Chern insulator. In particular, we can use this approach to clarify how the usual algorithms for constructing Wannier functions break down as one crosses into the Chern-insulator region of the phase diagram. Using numerical calculations on finite and periodic samples, we find that the total spread Ω of the maximally-localized Wannier functions [2] diverges for Chern insulators. However, its gauge-invariant part Ω_I, related to the localization length of Resta and Sorella [3], is finite in both insulating phases and diverges as the phase boundary is approached, as depicted in Fig. b. Furthermore, we find that the usual Wannier-function construction is bound to fail in Chern insulators because of singularities that appear in overlap matrices in both the real-space finite-sample and **k**-space extended-sample approaches. In addition, we find that the density matrix has exponential decay in both insulating phases, while having a power-law decay, more characteristic of a metallic system, precisely at the phase boundary [4].



a)



b)

a) Phase diagram of the Haldane model as a function of the model parameters φ and Δ/t_2. For our study we have chosen to cross into the Chern insulator phase along the vertical line at $\varphi = 1/4$. **b)** Gauge-independent part Ω_I and gauge-dependent part $\tilde{\Omega}$ of the spread $\Omega = \Omega_I + \tilde{\Omega}$ for different dense **k**-point meshes. The divergence is clearly visible at $\Delta/t_2 \approx 3.67$.

[1] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).

[2] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12847 (1997).

[3] R. Resta and S. Sorella, Phys. Rev. Lett. **82**, 370 (1999).

[4] T. Thonhauser and David Vanderbilt, Phys. Rev. **B** 74, 235111 (2006).