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Fermi-Surface Evaluation of Anomalous Hall Conductivity using Wannier Interpolation XINJIE WANG, DAVID VANDERBILT, Rutgers University, JONATHAN YATES, IVO SOUZA, LBNL and University of California, Berkeley — Recently, Haldane showed that the nonquantized part of the intrinsic anomalous Hall conductivity (AHC) can be represented as a Fermi-surface property.[1] The time-consuming integration of the Berry curvature over the entire Brilliouin zone is thereby converted into a more efficient integral over the Fermi surface only. Here we present an ab-initio approach for computing the AHC which combines a Haldane-like strategy with Wannier interpolation of the Bloch functions. First, a conventional electronic-structure calculation is performed and maximally-localized Wannier functions are constructed by a post-processing step, in order to transform the full ab-initio problem into an "exact" tight-binding form. Second, the Brilliouin zone is sampled by a large number of equally spaced parallel slices oriented normal to the total magnetization. We find the intersections of each Fermi surface sheet with every slice, organize these into a set of closed loops, and compute the Berry phase of the Bloch states as they are transported around these loops. The AHC is then just proportional to the sum of the Berry phases of all the loops on all the slices. The method is used to calculate the intrinsic AHC of Fe, Co and Ni.

[1]F.D.M. Haldane, Phys. Rev. Lett. **93** 206602 (2004).

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