Wannier interpolation for calculation of anomalous Hall conductivity in ferromagnets

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In the Hall effect a voltage develops in a metal plate in response to crossed electric and magnetic fields. In ferromagnets a Hall voltage exists even without an applied magnetic field. This puzzling phenomenom is the anomalous Hall effect. It results from a little-known term in the equations of motion of wavepackets in crystals, which can be thought of as a "megnetic field" in k-space and is a manifestation of Berry's phases in crystals. Recently, a first-principles calculation of the anomalous Hall conductivity (AHC) of iron as a Brillouin-zone integral of the Berry curvature was carried out and found to be in reasonable agreement with experimental results.[1] However, the authors observed extraordinarily strong and rapid variations of the Berry curvature with wavevector $\vec{k}$ in the vicinity of avoided crossings and near-degeneracies in reciprocal space. An extremely dense sampling of the Brillouin zone is therefore needed, rendering a conventional first-principles calculation rather time-consuming. Here, we present an efficient first-principles approach for computing the AHC based on Wannier interpolation. First, a conventional electronic-structure calculation is performed for Fe, on a relatively coarse k-point mesh. Second, maximally-localized Wannier orbitals are constructed by a post-processing step,[2] thus transforming the full ab-initio problem into an effective tight-binding form. Finally, the needed quantities such as Berry potentials and curvatures are interpolated onto a fine k-point mesh and used to compute the AHC. Our approach gives good agreement with conventional, less efficient first-principles calculations.

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[2] I. Souza, N. Marzari, and D. Vanderbilt, Phys. Rev. B **65**, 035109 (2001).