Dependence of anomalous Hall effect on spin-orbit coupling strength in bcc Fe

Xinjie Wang\textsuperscript{1}, Jonathan Yates\textsuperscript{2,3}, Ivo Souza\textsuperscript{2,3}, and David Vanderbilt\textsuperscript{1}

\textsuperscript{1}Department of Physics and Astronomy, Rutgers University
Piscataway, NJ 08854-8019
\textsuperscript{2}Department of Physics, University of California
Berkeley, CA 94720
\textsuperscript{3}Materials Science Division, Lawrence Berkeley Laboratory
Berkeley, CA 94720

Recently, a first-principles calculation of the anomalous Hall conductivity (AHC) of Fe as a Brillouin-zone integral of the Berry curvature was carried out and found to be in reasonable agreement with experimental results.\textsuperscript{1} However, these authors observed extraordinarily strong and rapid variations of the Berry curvature with wavevector \( k \) in the vicinity of avoided crossings and near-degeneracies in reciprocal space. Since the AHC vanishes in the limit of zero spin-orbit (SO) coupling, it is interesting to understand the behavior of the AHC as the SO coupling strength is artificially varied. We investigate this question working in the context of a Wannier interpolation approach to the calculation of the bandstructure and the AHC. The SO coupling strength is varied by tuning the projectors and their coefficients in the fully relativistic norm-conserving pseudopotential, which takes the form of a spatially-dependent \( 2 \times 2 \) matrix acting on spinor wavefunctions. In this way we separately control the strength \( \lambda_z \) of the spin-diagonal components and that of the spin-off-diagonal components \( \lambda_{xy} \) of the pseudopotential. The calculated AHC is found to be an odd function of \( \lambda_z \) and an even function of \( \lambda_{xy} \), with both linear and quadratic components playing a significant role in both cases. The existence of a contribution scaling as \( |\lambda_{xy}| \) is surprising from the viewpoint of conventional perturbation theory.