Wannier Interpolation of the Covariant Derivative of Berry Curvature and Orbital Moment.

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Abstract: The derivatives of the Berry curvature $\boldsymbol{\Omega}$ and intrinsic orbital magnetic moment m of the Bloch states arise in multiple problems, such as the nonlinear anomalous Hall effect [1] and magneto-transport within the Boltzmann-equation formalism [2] To study these properties in real materials, we developed a Wannier interpolation scheme for evaluating $\boldsymbol{\nabla}\mathbf{k}\boldsymbol{\Omega}$ and $\boldsymbol{\nabla}\mathbf{km}$ from first principles. We divide the wannierized energy bands in two groups ("in" and "out") based on a certain energy, and derive a gauge-covariant "generalized derivative" of the non-Abelian $\boldsymbol{\Omega}$ and m matrices defined over the inner states of interest. Unlike the simple derivative, the generalized derivative only involves couplings with the outer states, and preserves the gauge covariance of the $\boldsymbol{\Omega}$ and $\mathbf{m}$ matrices. This formulation leads to robust "Fermi-sea" formulas for the Berry curvature dipole[1] and kinetic magnetoelectric effect tensor [2], which converges much faster with the density of the integration $\mathbf{k}$-grid than the "Fermi-surface" formulas implemented earlier [3] in the Wannier90 code [4].

The implementation is done in our newly-developed code Wannier-Berri[5]. As a quick way to check the validity of the formalism, it was implemented for a two-band model (Haldane model). We compared the analytical derivatives with the numerical approximation, finding a good agreement between the two. In order to work with tight-binding models, we used the package PythTB [6].

[1] Sodemann, Inti. Physical review letters 115.21 (2015): 216806.

[2] Zhong, Shudan. Physical review letters 116.7 (2016): 077201.

[3] Tsirkin, Stepan S. Physical Review B 97.3 (2018): 035158.

[4] Pizzi, Giovanni. Journal of Physics: Condensed Matter 32.16 (2020): 165902.

[5] https://github.com/stepan-tsirkin/wannier-berri

[6] https://www.physics.rutgers.edu/pythtb