

Gauge-discontinuity contribution to Chern-Simons orbital magnetoelectric coupling

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A quantity that is closely related to the physics of topological insulators is an isotropic contribution to the orbital magnetoelectric coupling that is known as the “Chern-Simons” or “axion” or “ θ coupling” term. This last name comes from the fact that this contribution can be written in the form $(e^2/h)(\theta/2\pi)$, where θ is a phase angle, i.e., is only gauge-invariant modulo 2π . We propose here a new method for calculating θ , which is defined as a 3D Brillouin-zone integral of the Chern-Simons 3-form defined in terms of occupied Bloch functions. However, a straightforward finite-difference evaluation of this formula is only practical if a smooth and periodic gauge has been chosen in the entire Brillouin zone. Moreover, previous calculations have shown that for interesting systems expected to exhibit a large θ , such as topological insulators and systems derived from them, it is very difficult to converge the results with respect to \mathbf{k} -point sampling.

In order to solve this problem, we divide the Brillouin zone into subvolumes, and the gauge is chosen to be smooth within each subvolume. These subvolumes meet at 2D planes in \mathbf{k} -space where there is gauge discontinuity. The total θ response is then divided into contributions of two kinds: 3D integrals of the Chern-Simons 3-form over the subvolumes, and 2D integrals of a planar contribution associated with the gauge discontinuities on the boundary planes. Furthermore, in some cases it is necessary to subdivide the boundary planes into subregions separated by “vortex loops,” which make yet a third contribution in terms of Berry phases defined around the vortex loops. The total θ thus consists of three kinds of terms, expressed as integrals over 3D, 2D and 1D manifolds. Interestingly, in the presence of time-reversal (TR) symmetry, both the 3D and 2D integrals vanish (assuming the gauge has been chosen to respect TR symmetry), and the 1D vortex-loop integral is either 0 or π , corresponding to the \mathbb{Z}_2 classification of 3D time-reversal invariant insulators. We illustrate our method by applying it to the Fu-Kane-Mele model with applied staggered Zeeman field.