Topological Order in Electronic Wavefunctions

R. Resta

Dipartimento di Fisica, Università di Trieste, Trieste, Italy.

The geometrical and topological properties of electronic wave functions are commonly addressed in terms of the Berry connection and Berry curvature, both defined in some parameter space. The integral of the curvature over a closed surface equals 2π times an integer $C \in \mathbb{Z}$, called the (first) Chern number. C is measurable, in principle with infinite accuracy: 10^{-9} has been attained for the quantum Hall effect. Different values of C characterize topologically distinct electronic states; C is a topological invariant, extremely robust under changes in material parameters. The corresponding physical property is "topologically protected": in insulators the C value can be switched only passing through a metallic state. A $C \neq 0$ value requires absence of time-reversal symmetry.

For a crystalline insulator of noninteracting electrons the relevant parameter is the Bloch vector $\mathbf{k}$, the Berry curvature is the imaginary part of the Marzari-Vanderbilt metric, and the closed surface is the Brillouin zone (a torus). The paradigmatic systems are two-dimensional. I will illustrate two nonconventional approaches which can also cope with noncrystalline systems (disordered or macroscopically inhomogeneous). I will show how, in both approaches, C is evaluated avoiding any $\mathbf{k}$-integration. The rationale is that the topological order measures the entanglement of the ground state in the bulk of the sample. The k vector is an artificial construct: all ground state properties-including topological order–are embedded in the ground state density matrix, "shortsighted" in insulators.

The first approach [1] adopts periodic boundary conditions in a supercell framework, where the ground state is obtained from a single Hamiltonian diagonalization at $\mathbf{k} = 0$. The Berry curvature is defined as a response of the electronic wave function to an infinitesimal $\mathbf{k}$ change. For a large enough supercell, the value of the curvature at $\mathbf{k} = 0$ is enough to yield C: the major result is that it is computed with no extra diagonalization.

The second approach [2] introduces a topological marker, defined in $\mathbf{r}$ space, and which may vary in different regions of the same sample. Notably, this applies equally well to periodic and open boundary conditions. Simulations over a model Hamiltonian validate our theory. Our test cases include crystalline as well as disordered samples, and heterojunctions.

While the search for $C \in 0$ materials in zero $\mathbf{B}$ field is controversial, new classes of time-reversal symmetric topological insulators were predicted and discovered recently. Therein a novel two-valued invariant ($\mathbb{Z}_2$) discriminates topological order. Even the $\mathbb{Z}_2$ invariant can be defined and computed via integrals of the connection and curvature in $\mathbf{k}$ space, while no approach is available to cope with inhomogeneous systems (e.g. heterojunctions).

Partly funded by ONR Grant N00014-11-1-0145.

[1] D. Ceresoli and R. Resta, Phys. Rev. B **76**, 012405 (2007).

[2] R. Bianco and R. Resta, Phys. Rev. B **84**, 241106 (R) (2011).

Contact: resta@democritos.it