Orbital magnetization in periodic solids and its connection to NMR

Timo Thonhauser
Department of Physics and Astronomy, Rutgers University

A complete description of magnetism in solids requires not only the spin degrees of freedom, but also the "orbital magnetization." Despite the recent surge of interest in magnetic materials, it is quite surprising that the theory of orbital magnetization has remained in a condition similar to that of the polarization before the early 1990s, when the problem of computing finite polarization changes was solved by the introduction of the Berry-phase theory.[1] The essential difficulty, that the matrix elements of the position operator $\mathbf{r}$ are not well-defined in the Bloch representation, could be overcome by reformulating the problem in the Wannier representation. In order to derive an analogous theory for the orbital magnetization, we again work in the Wannier representation and assume a periodic insulator with broken time-reversal symmetry, vanishing (or commensurate) magnetic field, and zero Chern numbers. We show that a naive replacement of the dipole operator $\mathbf{r}$ by the circulation operator $\mathbf{r} \times \mathbf{v}$ in the expectation value of a bulk Wannier function gives only one contribution to the magnetization, i.e., the magnetization associated with the internal circulation of bulk-like Wannier functions. The missing contribution arises from net currents carried by the Wannier functions at the boundary of the sample. We prove that both contributions can be expressed as bulk properties in terms of Bloch functions in a gauge-invariant way.[2,3] With this new formalism at hand, I will then outline a possible approach for computing NMR shielding tensors via the orbital magnetization.

[1] R.D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993).

[2] T. Thonhauser, Davide Ceresoli, David Vanderbilt, and R. Resta, Phys. Rev. Lett. **95**, 137205 (2005).

[3] D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta Phys. Rev. B **74**, 024408 (2006).