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Orbital Magnetization in Periodic Insulators[1]

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Recent years have seen a surge of interest in issues of charge and spin transport in magnetic materials and nanostructures, including anomalous Hall and spin Hall effects. In this context, 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.[2] The essential difficulty, that the matrix elements of the position operator **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 analogue 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 by replacing the dipole operator **r** with the circulation operator $\mathbf{r}\times\mathbf{v}$, only one contribution to the magnetization is found, 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.[3] Our expression for the orbital magnetization is verified by comparing numerical tight-binding calculations for finite and periodic samples. Possible extensions to metals or insulators with non-zero Chern numbers will also be discussed.

[1]In collaboration with Davide Ceresoli, David Vanderbilt, and R. Resta.
[2]R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993).
[3]T. Thonhauser, Davide Ceresoli, David Vanderbilt, and R. Resta, Phys. Rev. Lett. **95**, 137 205 (2005).