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Orbital magnetization as a ground-state bulk property RAFFAELE RESTA, INFM Democritos National Simulation Center and University of Trieste, Italy, DAVIDE CERESOLI, TIMO THONHAUSER, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA — The magnetic dipole moment of any finite sample is well defined, while it becomes ill defined in the thermodynamic limit, due to the unboundedness of the position operator. Effects due to surface currents and to bulk magnetization are not easily disentangled. The corresponding electrical problem, where surface charges and bulk polarization appear as entangled, has been solved about one decade ago by the modern theory of polarization, based on a Berry phase. We follow a similar path here, providing a bulk expression for orbital magnetization for any lattice-periodical, though time-reversal breaking, Hamiltonian. We therefore limit ourselves to cases where the macroscopic (i.e. cell-averaged) magnetic field vanishes. For crystalline insulators we express the bulk magnetization in terms of Wannier functions, and we then transform the expression into a Brillouin-zone integral involving the occupied Bloch orbitals. The gauge-invariance of the final expression is explicitly shown. Interestingly, the final expression remains well-defined even for metals, but it is not yet clear whether it is correct in that case.

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