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Orbital Magnetization

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Microscopic understanding of what orbital magnetization M really is started only in 2005-6. The macroscopic current density responsible for M in a magnetized large sample is localized near its boundary, and therefore is lost in the idealization of an unbounded crystal, as customary in condensed matter physics. The modern theory avoids addressing currents altogether, and provides an alternative expression in terms of the Hamiltonian and of the ground-state electron distribution.

The founding work of 2005-6 addresses crystalline systems and provides the M expression in terms of k integrals of Bloch-orbital matrix elements: these clearly refer to unbounded samples. More recent work addresses instead bounded samples in r -space and shows that the M value can be retrieved without accessing the boundary currents: knowledge of the Hamiltonian and of the electron distribution in the bulk region of the sample is enough. Remarkably, this applies to both insulators [1] and metals [2].

The modern theory provides M as the sum of two terms, both gauge invariant. The quantity actually measured in magnetic circular dichroism experiments is only one of the two terms, not the full M value [3].

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- [2] A. Marrazzo and R. Resta, Irrelevance of the boundary on the magnetization of metals, Phys. Rev. Lett. 116, 137201 (2016).
- [3] I. Souza and D. Vanderbilt, Dichroic f -sum rule and the orbital magnetization of crystals, Phys. Rev. B 77, 054438 (2008).

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