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Optical sum rules for the orbital magnetization and anomalous Hall conductivity

IVO SOUZA, Dept. of Physics, University of California Berkeley

Magnetic circular dichroism (MCD), the differential absorption of left- and right-circularly-polarized light by ferromagnets, results from the interplay between spin polarization and spin-orbit interaction. The same two ingredients are responsible for their spontaneous ("anomalous") Hall conductivity (AHC) and orbital magnetization. I will discuss how the three phenomena are related by two sum rules for the interband MCD spectrum.[1] The sum rules are of the form $\int_0^\infty \omega^{-p}\sigma''_{\mathrm{A},\alpha\beta}(\omega)d\omega$, where σ''_{A} is the absorptive part of the antisymmetric optical conductivity. The sum rule with $p=0$ is the dichroic counterpart of the familiar f-sum rule for linearly-polarized light. I will show that it yields a contribution to the ground-state orbital magnetization which in insulators is associated with the circulation of the Wannier orbitals around their centers (more precisely, to the gauge-invariant part thereof). This differs from the net circulation, or total orbital magnetization,[2,3] which has two additional contributions: (i) the remaining Wannier self-rotation, and (ii) the "itinerant" circulation arising from the center-of-mass motion of the Wannier orbitals. Contributions (i) and (ii) are not separately meaningful, since their individual values depend on the particular choice of Wannier functions. Their sum is however gauge-invariant, and can be inferred from a combination of gyromagnetic and magneto-optical experiments. The $p=1$ sum rule is the dc limit of the dichroic Kramers-Kronig relation which yields $\sigma'_{\mathrm{A}}(0)$, the Karplus-Luttinger AHC. *Ab-initio* studies have shown that it is necessary to sample over millions of k-points to converge the calculation of this quantity. I will describe an efficient real-space method for computating the AHC[4] and MCD[5] using Wannier functions, and present some illustrative calculations for ferromagnets as well as field-polarized solid and liquid heavy metals.[6] The possible role of configurational disorder in enhancing the field-induced AHC of liquid metals by introducing low-frequency Drude-related features in the MCD spectrum will be explored.

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