# Transport properties calculated by means of the Kubo formalism and using the spin-polarized relativistic KKR-CPA method

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Many physical phenomena exploited in spintronics can be described by means of a corresponding linear response tensor. Kubo's response formalism provides a firm and powerful basis to determine the response of a solid to a perturbation in a very general way. A first-principles approach is presented that is based on the corresponding Kubo-Bastin equation [1] and implemented within the fully relativistic KKR (Korringa-Kohn-Rostoker) formalism [2]. This approach is able to treat intrinsic and extrinsic contributions on equal footing. Both contributions from states below (*Fermi sea*) and at the Fermi level (*Fermi surface*) are treated and can be analyzed in detail. The approach is applicable to pure systems as well as metallic and semiconductor alloy systems with disorder accounted for by means of the CPA (Coherent Potential Approximation). Special emphasis is put on the role of the so-called vertex corrections that allow to build a bridge to the semi-classical Boltzmann transport formalism [3]. Several examples (anomalous Hall and anomalous Nernst [4] as well as spin Hall and spin Nernst [5] conductivities, as well as spin-orbit torque [6]) are given to illustrate this analysis in combination with numerical results obtained using the spin-polarized KKR electronic structure method. As a new feature in this type of numerical studies the inclusion of finite temperature effects as lattice vibrations and spin fluctuations will be discussed. The approach [7] is based on the alloy analogy model with thermal vibrations and spin fluctuations modeled by random atomic displacements and tilting of magnetic moments, respectively. Various models to deal with spin fluctuations and their impact on the temperature dependent behavior of the electrical conductivity and Gilbert damping parameter will be discussed. The corresponding results demonstrate in particular the non-additivity of the separate contributions to the conductivity.

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