Electronic and spin transport within the Kubo Formalism - a relativistic Green function KKR approach

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Starting from Kubo linear response theory a general approach to describe various transport phenomena from first-principles is presented.

We employ a fully relativistic KKR framework in a spin-density functional formulation which allows treating the full (spin-) conductivity tensor including its antisymmetric components and thereby spin-orbit induced transverse transport phenomena like the spin- and anomalous Hall effects. Kubo-Streda and Kubo-Bastin approaches have been implemented with the latter treating both, Fermi-sea and Fermi-surface terms on the same footing. Employing the coherent potential approximation leads to a description of disordered alloys through the whole concentration range. Intrinsic as well as extrinsic contributions are fully accounted for. The role of vertex corrections and their importance will be discussed. The inclusion of finite temperatures and the extension of the formalism to treat spincaloritronic phenomena is presented. Applications to transition-metals and their alloys demonstrate the versatility of the method.

1. Wimmer, Ködderitzsch, Ebert, PRB 89 (R), 161101 (2014)
7. Lowitzer, Ködderitzsch, Ebert, PRL 105, 266604 (2010)