First-principles scattering matrices for spin-transport

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Details are presented of an efficient formalism for calculating transmission and reflection matrices from first principles in layered materials. Within the framework of spin density functional theory and using tight-binding muffin-tin orbitals, scattering matrices are determined by matching the wave-functions at the boundaries between leads which support well-defined scattering states and the scattering region. The calculation scales linearly with the number of principal layers N in the scattering region and as the cube of the number of atoms H in the lateral supercell. For metallic systems for which the required Brillouin zone sampling decreases as H increases, the final scaling goes as H^2N. In practice, the efficient basis set allows scattering regions for which $H^2N \sim 10^6$ to be handled. The method is illustrated for Co/Cu multilayers and single interfaces using large lateral supercells (up to 20 x 20) to model interface disorder. Because the scattering states are explicitly found, "channel decomposition" of the interface scattering for clean and disordered interfaces can be performed. Other discussed applications of the method include anisotropy of interface scattering, spin-transfer and spin-injection.

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