Ab-initio theory of ultrafast laser-induced demagnetization

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More than a decade ago it was discovered that excitation of a metallic ferromagnet with an intensive femtosecond laser-pulse causes an ultrafast demagnetization within 300fs [1]. Until today, the mechanism(s) underlying the fs demagnetization could not be uncovered and remain a controversial issue. Several theories have been proposed – mostly based on the assumption that there must exist an ultrafast channel for the dissipation of spin angular momentum. One of the proposed fast spin-flip channels is the Elliott-Yafet electron-phonon spin-flip scattering [2].

We probe several of the proposed mechanisms using ab-initio caluclations. To examine the electron-phonon spin-flip scattering we compute ab-initio the spin-flip Eliashberg function, from which we calculate the spin-flip probability and demagnetization for various situations, viz. equilibrium distributions, hot electron distributions in the thermalized regime, and laser-induced non-equilibrium conditions [3]. Hot electron distributions in the electron-thermalized regime are calculated to lead only to a very small demagnetization rate. A larger net demagnetization is computed for laser-induced non-equilibrium conditions, however, also this contribution is not sufficient to explain the measured fs demagnetization. Following a different rationale we have developed a model for fs laser-induced magnetization dynamics, based on the high mobility of laser-excited spin-polarized electrons [4]. We establish the influence of fast electron dynamics of excited non-equilibrium electrons and show that this provides spin-transport in the super-diffusive regime, causing effectively a demagnetization. We find that super-diffusive flow of hot electrons can account for the experimentally observed demagnetization within 200fs in Ni.

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