Ultrafast magnetism within Time Dependent Density Functional Theory

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The search for practical solutions to increase the speed of manipulation of magnetic bits is a very important problem in modern information technology. Since the outstanding discovery of the demagnetization of a Ni film by a 60 femtosecond optical laser pulse [1] several theoretical models have been proposed. In the literature possible explanations involve spin losses due to direct coupling between laser photons and the electron spins, superdiffusive and electron phonon scattering mechanisms.

In this work we want to show how the ultrafast demagnetization process can be explained just in terms of an interaction between the electronic and the spin degrees of freedom of the system. Using the time dependent extension of Spin Density Functional Theory we have investigated the magnetization dynamics of ferromagnetic and antiferromagnetic transition metal systems. The results show that the demagnetization is initially driven by the pulse and then decays towards a new equilibrium state, furthermore, the effect is strongly dependent on the initial magnetic configuration of the crystal. We finally present a model where the spin loss arises naturally as a consequence of the far from equilibrium interplay of the electronic and the spin subsystems.