How to demagnetize a ferromagnetic solid with a short laser pulse, and how to enhance a single peak in the harmonic spectrum: Some answers given by TDDFT

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After a pedagogical introduction to time-dependent density-functional theory (TDDFT), two recent applications of the theory will be presented:

(i) We study the laser-induced ultrafast demagnetization of solid Fe, Co and Ni, using the non-collinear spin-dependent version of TDDFT. We show [1] that the demagnetization proceeds in two distinct steps: First, a fraction of the electrons is excited whithout much change in the spin polarization of the system. In the second step, the spin magnetic moment of the remaining localized electrons decreases through spin-flip transitions. This process is induced by spin-orbit coupling; when spin-orbit coupling is switched off, the moment stays constant in time. The whole process of demagnetization happens in less than 50 femto-seconds.

(ii) In the second application we search for laser pulses that allow the enhancement of a single peak in the harmonic spectrum of H or He. We achieve an enhancement of 2-3 orders of magnitude in the single-atom response (i.e. not through phase matching). To calculate the optimized pulses we combine [2] TDDFT with optimal control theory.

1. K. Krieger, J.K. Dewhurst, P. Elliott, S. Sharma, E.K.U. Gross, arXiv:1406.6607 [cond-mat.mtrl-sci](2014).

2. A. Castro, J. Werschnik, E.K.U. Gross, PRL 109, 153603 (2012).