

MAR08-2007-002163

Abstract for an Invited Paper
for the MAR08 Meeting of
the American Physical Society

First-principles approach to Non-Collinear Magnetism: towards Spin Dynamics

E.K.U. GROSS, Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195, Germany

Most formulations of spin density functional theory (SDFT) restrict the magnetization vector field to have global collinearity. Nevertheless, there exists a wealth of strong non-collinearity in nature, for example molecular magnets, spin-spirals, spin-glasses and all magnets at finite temperatures. The local spin density approximation (LSDA) can be extended to these non-collinear cases [1] but this extension has the undesirable property of having the exchange-correlation (xc) field parallel to the magnetization density at each point in space. When used in conjunction with the equation of motion for the spin magnetization in the absence of spin currents and external fields [2,3], this local collinearity eliminates the torsional term, resulting in no time evolution. This severe shortcoming of LSDA, where the physical prediction is qualitatively wrong, opens up an important new direction for the development of functionals where this time evolution is correctly described. Towards this goal, I will describe our extension of the Kohn-Sham optimized effective potential (OEP) method to the non-collinear case and derive the corresponding integral equations, applicable to both finite and extended systems [3,4]. Most importantly I'll show that the resulting magnetization and xc field are not locally collinear to each other for real solids, and will therefore produce manifestly different spin-dynamics.

[1] J. Kuebler, K.-H. Hoek, J. Sticht and A. R. Williams, *J. Phys.* **F18**, 469 (1993).

[2] K. Capelle, G. Vignale and B. L. Gyorffy, *Phys. Rev. Lett.* **87**, 206403 (2001).

[3] S. Sharma, J. K. Dewhurst, C. Ambrosch-Draxl, S. Kurth, N. Helbig, S. Pittalis, S. Shallcross, L. Nordstroem and E.K.U. Gross *Phys. Rev. Lett.* **98**, 196405 (2007)

S. Sharma, S. Pittalis, S. Kurth, S. Shallcross, J. K. Dewhurst and E.K.U. Gross *Phys. Rev. B* **76**, 100401 (Rapid Comm.) (2007)