Seminar on Condensed Matter Theory

Group of Theoretical Physics at the Department of Condensend Matter Physics
of Charles University has a pleasure to invite you to attend the seminar

on 20 September 2018 at 14:00

at Faculty of Mathematics and Physics of Charles University, Ke Karlovu 5, 121 16 Praha 2

Seminar room F052

Dr. Lars Bergqvist

KTH Royal Institute of Technology, Stockhom, Sweden

General method for atomistic spin-lattice dynamics with first principle accuracy

We present a computationally efficient general first-principles based method for spin-lattice simulations for solids and clusters. The method is based on a coupling of atomistic spin dynamics and molecular dynamics simulations, expressed through a spin-lattice Hamiltonian, where the bilinear magnetic term is expanded up to second order in displacement. The effect of first order spin-lattice coupling on the magnon and phonon dispersion in bcc Fe is reported as an example, and we observe good agreement with previous simulations. In addition, we also illustrate the coupled spin-lattice dynamics method on a more conceptual level, by exploring dissipation-free spin and lattice motion of small magnetic clusters (a dimer, trimer and quadmer). The here discussed method opens the door for a quantitative description and understanding of the microscopic origin of many fundamental phenomena of contemporary interest, such as ultrafast demagnetization, magnetocalorics, and spincaloritronics.

For more information follow: theory.kfkl.cz/seminars.php
If you wish to receive regular updates on fothcoming seminars, contact T. Novotný (tno@karlov.mff.cuni.cz).