MATERIALS IN MAINZ SCIENCE

Technical Training: Theory

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

A Mini-Course on Computer Simulation Methods in Condensed Matter Physics

Dates: September 3, September 17 and September 18, 2014

Time: 9-11am (c.t.)

Location: MAINZ Seminar Room, Staudinger Weg 9, 3rd floor, room number 03-122

Speaker: Prof. David Landau (University of Georgia; MAINZ Visiting Professor 2013)

September 3, 2014

Lecture 1: Introduction to atomistic simulations in statistical physics

In all but the smallest systems of interacting atoms and molecules, the huge number of possible states renders exact solution almost always impossible. Instead, atomistic simulations methods implemented on modern computational resources offer impressive and powerful alternatives. Several well developed simulational methods, including molecular dynamics (MD), Monte Carlo (MC) and spin dynamics (SD) will be introduced. Algorithmic features and the relative merits and limitations of the different approaches will be discussed.

September 17, 2014

Lecture 2: Critical endpoint behavior in an asymmetric Ising model: Application of Wang-Landau sampling

Using the Wang-Landau sampling method with a two-dimensional random walk, we determine the density of states for an asymmetric Ising model with two- and three-body interactions on a triangular lattice in the presence of an external field. (This model can be used to describe systems with coexisting liquid or alloy phases.) With an accurate density of states we map out the full phase diagram and perform quantitative finite-size analyses at, and away from, the critical endpoint. We observe a clear divergence of the curvature of the spectator phase boundary and of the magnetization coexistence diameter derivative at the critical endpoint and find that the exponents for both divergences agree well with previous theoretical predictions.

September 18, 2014

Lecture 3: Spin-wave multiple excitations in nanoscale classical Heisenberg antiferromagnets.

Spin dynamics simulations of a nanoscale, classical, Heisenberg antiferromagnet on a simple cubic lattice at a temperature below the Neel temperature are presented. Nanoparticles and nanofilms are modeled and results are compared to those for the “infinite” system with periodic boundary conditions. The local dynamic structure factor $S^T(q,\omega)$ was calculated from the local space- and time-displaced spin-spin correlation function. Multiple excitation peaks for wave vectors within the first Brillouin zone appear in the spin-wave spectra of the transverse component $S^T(q,\omega)$ but are lacking if periodic boundary conditions are used. Assuming q-space spin-wave reflections with broken momentum conservation due to free-surface confinements, we explained those spectra quantitatively in the linear dispersion region.