Master research project
Quantum Monte Carlo simulations of
Peierls and CDW phases in quantum wires

Eric Jeckelmann
Institut für Theoretische Physik
Leibniz Universität Hannover

September 9, 2011

Motivation

This master project is a contribution to a larger research project on the electronic properties of nanowires. It is part of the proposed DFG Research Unit "Metallic nanowires on the atomic scale: Electronic and vibrational coupling in real world systems" (FOR-1700) and will be carried out in collaboration with other members of this Research Unit. The properties of nanowires are different from those of ordinary solids because of their quasi-one-dimensional geometry. It is well known that the Coulomb interaction between electrons and the coupling between electrons and phonons can lead to spontaneous-broken-symmetry phases in quantum wires, such as Peierls and CDW ordered insulating states. However, strong quantum and thermal fluctuations influence the stability these phases decisively. Moreover, the role of the surface supporting the nanowires (substrate) is poorly understood.

Goal

The goal of this master research project is to investigate the emergence of Peierls and CDW broken symmetry phases in quantum lattice models representing a weakly-coupled array of quantum wires in a "vacuum" or on a substrate. In particular, this work should clarify the phase diagram and the nature of the phase transitions as a function of temperature and interchain coupling. The student will first perform analytical calculations of the model properties using mean-field approximations and perturbation theory to delimit the scope of the problem to be solved numerically. Then he/she will implement a quantum Monte Carlo (QMC) program to compute the thermodynamical properties of these models and carry out the QMC simulations.

Work plan

1. Analytical ground-state and finite-temperature calculations for several configurations (a single quantum wire, 2D/3D arrays of quantum wires, a single nanowire on a substrate, arrayed nanowires on a surface)
2. Implementation of the QMC program
3. QMC simulations of arrayed quantum wires in a "vacuum"
4. QMC simulations of a single nanowire on a substrate

References

1. Nanosystems: C.P. Poole Jr. and F.J. Owens, *Introduction to Nanotechnology*, Wiley 2003.
2. 1D materials: M. Springborg and Y. Dong, *Metallic Chains / Chains of Metals*, Elsevier 2007
3. Monte Carlo: R.H. Landau *et al.*, *A survey of computational physics*, Princeton University Press 2008
4. Monte Carlo: J.M. Thijssen, *Computational Physics*, 2nd ed., Cambridge University Press 2007