Institut für Theorie der Kondensierten Materie Institut für Nanotechnologie

Lecture announcement WS 2012/2013

Computational Condensed Matter Theory

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Lecture: Do 9:45-11:15. Practice: tba, (SWS: 2+1) KI. HS B, KIT, Campus South.

Requirements:

Lecture: basic quantum mechanics & solid state physics Practice: basics programming knowledge Literature: will be given in first lecture course

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The advent of powerful algorithms -- like the transfer-matrix method, numerical renormalization group schemes, Krylov-subspace methods, ...-together with the improving computer power has opened up a completely new route to test existing concepts and to obtain new insights into broad

classes of physical systems. Nowadays, computational tools are well established in all branches of theoretical physics and make unique and indispensable contributions. Indeed, often they provide the only route for systematic studies and improved understanding.

This lecture offers an introduction into basic computational techniques and the conceptual ideas behind. The pedagogical approach of the lecture will be to start from a fundamental physics example and then develop a numerical approach starting from there. In exercises practical implementations (e.g. with MatLab) will be given. Concepts of the lecture will be illustrated in terms of simple, but scientifically already meaningful examples.

The following topics will be addressed:

1. The gas of non-interacting fermions: tight binding models and their electronic structures

- 1.1 Excursion: Topologically non-trivial materials and graphene
- 1.2 Disorder effects: General purpose numerics
- 1.3 Wavepacket dynamics in nanostructures: Krylov subspace technology
- 2. Elements of transport theory

2.1 Anderson localization in dirty quantum wires: Transfer matrix methods

3. Fermi liquid corrections

- 3.1 Briefing: Fermi-Liquid-Theory
- 3.2 Hartree-Fock method
- 3.3 Working horse for electronic structure calculations: Density functional theory

4. Strongly correlated electron systems

- 4.1 Briefing: Kondo effect
- 4.2 The numerical renormalization group
- 4.3 Briefing: Luttinger liquid
- 4.4 The density renormalization group method



