Computational Methods for Correlated Quantum Systems

The following is the outline for 12 lectures by James Dufty (UF), Michael Bonitz, Karsten Balzer and Alexei Filinov (all Kiel, Germany) on theoretical concepts and practical tools to describe the structure and dynamics of quantum systems with strong correlations.

New time and place starting November 10: 10:40 AM – 11:30 PM, Room 2205

I. **Quantum potentials for semi-classical methods** (Dufty; Nov. 5,7)
   a) Examples of equilibrium and non-equilibrium classical – quantum mappings
   b) Pair potentials with diffraction and spin effects; degeneracy effects
   c) Wave packet molecular dynamics
   d) Orbital free density functional theory

II. **Classical and Path Integral Monte Carlo** (Filinov, Bonitz; Nov. 10,12,14, 17)
   a) Introduction to classical Metropolis Monte Carlo
   b) Quantum Statistics, Density matrix
   c) Feynman's path integral. Mapping onto an effective classical system
   d) Spin statistics, exchange, Fermion sign problem
   e) Generalized Metropolis algorithm for quantum systems, PIMC
   f) High-temperature N-particle density matrix
   g) Calculation of physical observables
   h) Simulation of macroscopic systems – finite size effects
   i) Applications: electrons in quantum dots, Fermi liquid and Wigner crystal,
   j) Bosons: Bose condensation, superfluidity

b) **Quantum Molecular Dynamics** (Filinov, Bonitz ; Nov. 19, 21)
   a) Equation of motion for the Wigner distribution
   b) Solution by an iteration series. Classical dynamics and quantum corrections
   c) Numerical implementation by Monte Carlo and MD techniques

c) **Quantum kinetic equations** (Bonitz, Balzer; Nov. 24, Dec. 1,3,5)
   a) Second quantization and real time (Keldysh) Green's functions
   b) Kadanoff-Baym/Keldysh equations.
   c) Selfenergy. Important Feynman Diagrams
   d) Single time kinetic equations (Boltzmann equation)
   e) Numerical procedure
   f) Numerical Results
   g) Interband Kadanoff-Baym equations
   h) Application to localized systems: quantum dots and atoms

References: "Introduction to Computational Methods for Many-Body Systems",
M. Bonitz and D. Semkat (eds.), Rinton Press, Princeton 2006
Starting date: November 5. No lecture November 26,28 (Thanksgiving on 27/11)