Rechnergestützte Physik I

WS 2001/02

Information

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- Web pages:
  - http://www.itp.phys.ethz.ch/lectures/RGP

Administrative issues

- Time of the lecture ?
- Time of the exercises?

- Computer accounts:
  - Distributed memory Beowulf Cluster „Asgard“
  - Shared memory parallel computer „Tornado“
  - Vector super computer Cray J-90
  - Sign up this week or next!

  - Student workstation accounts of the D-PHYS

About the course

- The RGP I course is a (recommended) prerequisite for
  - RGP II
  - Computational semester thesis

- RGP I and II are (recommended) prerequisite for
  - Computational diploma theses
  - Computational PhD theses

- Studiengang “Rechnergestützte Wissenschaften”
  - From the 5th Semester
  - Alternative to physics, more computer-oriented

Prerequisites

- Programming
  - Knowledge of at least one programming language
  - Basic algorithms
  - Fundamental data structures
    - Arrays, lists, trees
- Numerical analysis
  - Root solvers
  - Linear systems of equations and eigenvalue problems
  - Numerical integration and differentiation
  - Basic knowledge of statistics
- Physics
  - Classical mechanics and electrodynamics
  - Basics of statistical mechanics
  - Basics of quantum mechanics

Questions regarding programming

- Who knows
- C?
- Java?
- C++?
  - Classes?
  - Inheritance?
  - Templates?
  - Generic Programming?
  - Optimization in C++?
  - Expression templates?

Overview

- Rechnergestützte Physik I
  - Programming techniques for scientific computing
  - Super computing
  - Nuemrical analysis
  - Physics applications
  - Exercises taking 1-2 week each
  - Wahlfach for physicists, Vertiefungsfach and RW students
- Rechnergestützte Physik II
  - More algorithms
  - Many body problems
  - Error analysis
  - One long project as exercise
  - Wahlfach for physicists, Vertiefungsfach for RW students

More administrative details

- Students interested in a diploma or PhD thesis or in computational physics
- Either change to RW
- Or study theoretical physics
  - pick RGP I&II as “allgemeines Wahlfach”
  - Or as “mathematisches Wahlfach”
    - And any numerical analysis seminar from the math department

Rechnergestützte Physik I

- Programming
  - Object oriented programming
    - C++, Java
  - Generic programming
    - templates
  - Optimization: faster than FORTRAN?
  - Visualization
    - Java
- Supercomputing
  - Programming of parallel computers and Beowulf clusters
  - Programming of vector supercomputers
  - Optimization

Rechnergestützte Physik I

- Numerical analysis
  - Integration, differential equations
  - Matrix problems
  - Random numbers
  - Software libraries
- Applications
  - Mechanics
  - Electrodynamics
  - Population dynamics
  - Wave equation, heat equation, ...
  - Quantum mechanical one body problems

What you will learn

- All phases of a scientific simulation
  - Analysis of the problem
  - Development of a model
  - Searching for an algorithm
  - Implementation of the algorithm
    - Use of libraries
    - Generic and reusable implementation of new algorithms
  - Optimization
    - Optimization, vectorization, parallelization
  - Testing and debugging
  - Simulation
  - Error analysis
  - Writing a report

Literature on C++

- Stanley B. Lippman, *Essential C++,* Addison Wesley 2000
  - Good and short introduction
- Bjarne Stroustrup, *The C++ Programming Language*, 3rd edition, Addison Wesley 1997
  - The reference book
- Stanley B. Lippman and Josée Lajoie, *C++ Primer*, 3rd edition, Addison Wesley 1998
  - Good introduction, incomplete as reference
- John J. Barton and Lee R. Nackman, *Scientific and Engineering C++*, Addison Wesley 1994
  - outdated
- Articles on scientific C++ in
  - *Computers in Physics* (to 1998)
  - *IEEE Journal on Computing in Science and Engineering* (from 1999)

Literature on computational physics

- Harvey Gould und Jan Tobochnik
  An Introduction to Computer Simulation Methods,
  2nd edition, Addison Wesley 1996
  - Extensive introduction, also for non-physicists.
- Rubin H. Landau and Manual J. Paez,
  Computational Physics, John Wiley 1997
  - Good contents but not so good layout
- Tao Pang,
  An Introduction to Computational Physics,
  Cambridge University Press 1997
  - good but advanced, some typos
- Wolfgang Kinzel und Georg Reents,
  Physik per Computer, Spektrum Akademischer Verlag
  - Good introduction but little contents
- J.M. Thijssen,
  Computational Physics, Cambridge University Press 1999
  - The best book, but quite advanced

A first example

- Magnetic properties of planar antiferromagnets
  - Spin-1/2
    - La_2CuO_4
    - $Sr_2CuO_2Cl_2$
  - Spin-1
    - La_2NiO_4
    - K_2NiF_4
- Neutron scattering measurements of the correlation length
- Theoretical predictions
- Problem: they do not agree
  - Problem in experiment?
  - Problem in theoretical model?
  - Problem in analytical approximation?

From material to model

- As simple as possible but not simpler
- Layered material
  => Restriction to a plane
- Only $d_{x^2-y^2}$-electrons are magnetically active
  => Reduction to a single band model
- Strong Coulomb repulsion
  => purely magnetic model
- Simplest model is Heisenberg quantum antiferromagnet on a square lattice
- Quantum fluctuations are essential
  cannot simplify it to a classical model

Theoretical predictions I

- Mapping to the (2+1)D nonlinear σ model
  - Effective field theory:
  - better for larger spin *S*
  - Exact for *T*–> 0
- Renormalization group gives exact asymptotic behavior at low temperatures (CHN-HN)

$$\frac{\xi}{a} = \frac{e}{8}\frac{c/a}{2\pi\rho_s}\exp\left(\frac{2\pi\rho_s}{k_B T}\right)\left[1-\frac{k_B T}{4\pi\rho_s}+\ldots\right]$$

- The values of *c* and ρ_s are determined by the exchange coupling *J* of the Heisenberg model and can be measured independently

Theoretical predictions II

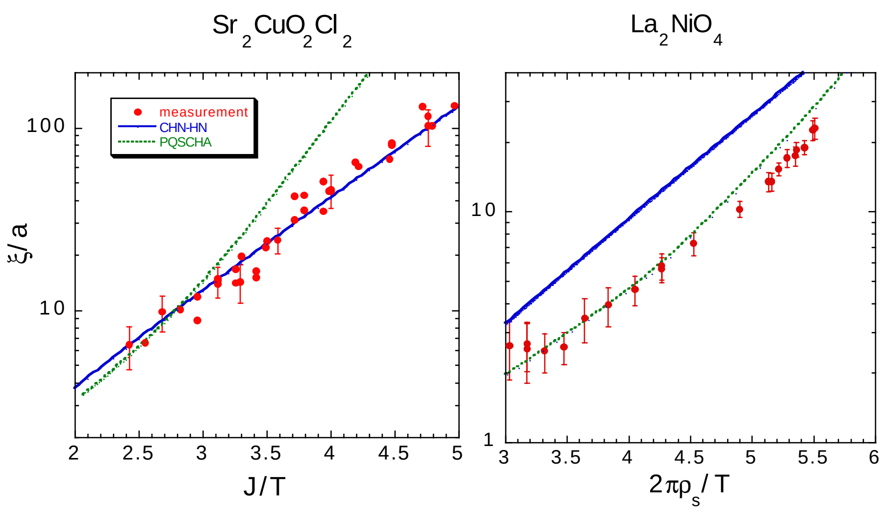
- Mapping to a classical model at renormalized temperature (PQSCHA)

$$\xi = \xi_{classical}(f_S(T))$$

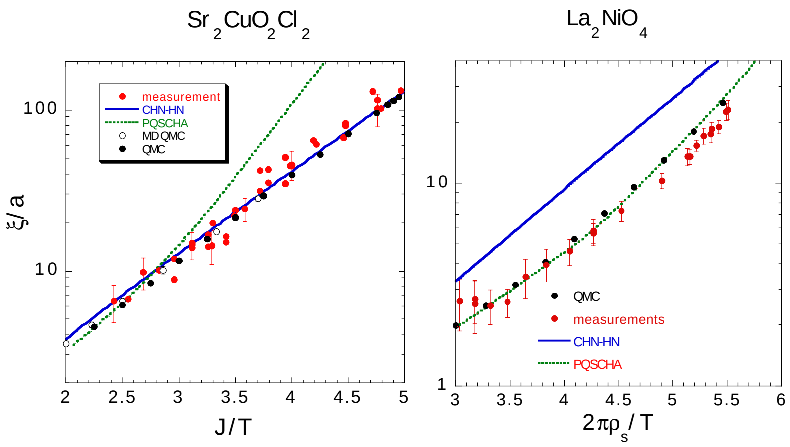
  - Harmonic approximation of the quantum fluctuationa: Pure Quantum Self Consistent Harmonic Approximation
  - Exact for T–> ∞
  - Incorrect for T–> 0

- The renormalization function f_S depends only on *S* and *J*. Both quantities are known

Experimental measurements



Simulation results



Simulation

- Is the model wrong?
  - No, QMC simulations agree?
- Are the theories wrong?
  - No
- How do we resolve the problems?
  - Different theories applicable for different regimes
  - Need numerical simulation to determine validity of theories