Computational Many-Body Physics

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Sheet 7: return on: Monday, July 18, 2016, 14:00

Exercise 1: the module exam

(15 bonus points)

As a preparation for the module exam, here are a few issues to think about:

a) What is the difference between single-particle and many-particle energies? (2 bonus points)

b) Consider the Hubbard model on a cluster with M sites. What are the physical properties and phenomena we are interested in? (3 bonus points)

c) The number of sites in b) should take the values $M = 5, 20, 50, 100, 1000$. Which (computational) method would you recommend for each of these values? (4 bonus points)

d) Explain the basic strategy of the NRG method (maximum one page). (3 bonus points)

e) What are the physical phenomena related to Kondo physics? (3 bonus points)

Exercise 2: feedback

(5 bonus points)

a) Which exercise did you like best? Explain your choice. (1 bonus point)

b) Which exercise did you find inappropriate, or useless, or too difficult, etc.? (1 bonus point)

c) Which exercise did you miss? Suggestions are welcome! (3 bonus points)

Exercise 3: Metropolis algorithm

(6 points)

In the Metropolis algorithm (as applied to the Ising model), random changes in the spin configurations are either accepted or rejected. It might appear strange that, if a change is rejected, the same spin configuration appears twice (or even three times etc.) in a row of the Markov chain. It is essential, however, that the unchanged spin configurations are included in the Markov chain to get the proper probability distribution. This can be analysed in a much simpler context: the application of the Metropolis algorithm to a one-dimensional integral.

Consider the one-dimensional integral

$$I = \int_{-\infty}^{\infty} \mathrm{d}x\, w(x) g(x) \ , \quad \text{with } w(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} \ .$$

The Metropolis algorithm generates a Markov chain of random numbers $\{x_i\}$, with a distribution given by $w(x)$, from which the integral can be approximated as

$$I \approx \frac{1}{N} \sum_{i=1}^{N} g(x_i) \ .$$

a) Implement an appropriate Metropolis algorithm and show that, indeed, the distribution of the random numbers $\{x_i\}$ is given by $w(x)$. (4 points)

b) What happens when we remove the unchanged x_i from the Markov chain? (2 points)

Exercise 4: truncation

(8 points)

The idea of this exercise is to find out in which cases the truncation of the states with highest energies (as done in the NRG) is justified. We consider the one-dimensional Heisenberg model with N sites, for which the ground state can be obtained with the programs developed in the previous exercises.

a) For $N = 6$, calculate the ground state $|\psi\rangle_{\mathrm{g}}$ of the Heisenberg model. The ground state can be written as

$$|\psi\rangle_{\mathrm{g}} = \sum_{ij} c_{ij} |i\rangle_{\mathrm{A}} |j\rangle_{\mathrm{B}} \ ,$$

with $|i\rangle_{\mathrm{A}}$ the basis of eigenstates of the Heisenberg model for the first three sites (part A) and $|j\rangle_{\mathrm{B}}$ accordingly for the remaining three sites (part B). Calculate the coefficients c_{ij} and analyse the dependence of c_{ij} on $E_{\mathrm{A},i} + E_{\mathrm{B},j}$. (5 points)

b) Repeat the analysis of part a) with a reduced value $|J'| < |J|$ for the coupling between the two parts. What happens in the limit $J' \to 0$. (3 points)