Computational Many-Body Physics

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SS 2020

Sheet 2 - please submit your solutions via e-mail to Chae-Yeun Park until Monday, May 18, 2020, 12:00.

Exercise 1: Metropolis algorithm

(7 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

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

The $\bar{x}_{i+1}$ in the Metropolis algorithm can be calculated as

$$\bar{x}_{i+1} = x_i + h\delta \ ,$$

with δ a random number between -1 and 1 (equally distributed). The maximum step size h can be set to $h = 1$.

a) Implement an appropriate Metropolis algorithm and show that, indeed, the distribution of the random numbers $\{x_i\}$ is given by $w(x)$. (5 points)

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

Exercise 2: Metropolis algorithm for the two-dimensional Ising model

(8 points)

In this exercise, we consider the Ising model in a magnetic field

$$H = -J \sum_{<ij>} S_i^z S_j^z - h \sum_i S_i^z,$$

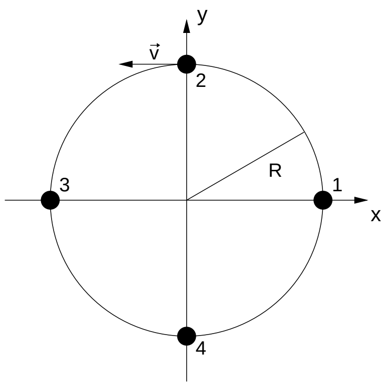
on a two-dimensional square lattice ($N \times N$) with coupling between nearest neighbours and periodic boundary conditions. The strength of the coupling can be set to $J = 1$ (the ferromagnetic case) and N can be set to $N = 64$.

a) Write a code which generates a Markov chain of 10000 spin configurations for a given temperature T, starting from a random spin configuration. In each iteration, the (possibly) new spin configuration is generated by flipping a *single* spin, as described in the script and in the lecture (Video No. 8). Plot the final spin configurations for temperatures $T = 0.1$, 0.5, 2.0, and 10.0 and magnetic field $h = 0$. (4 points)

b) Calculate the temperature dependence of the average magnetization for various values of h. (4 points)

Exercise 3: N-body gravitational systems in 2d

(13 points)



In this exercise, we consider a system of N bodies (with masses $m_i = m$, $i = 1, \ldots, N$), interacting via the gravitational force between the bodies. The bodies are moving in circular orbits with radius R as sketched in the above figure for $N = 4$. The velocities of the bodies have constant and equal magnitude: $|\vec{v}_i(t)| = v$.

a) Specify the orbits $\vec{r}_i(t)$, $i = 1, \ldots, N$, for arbitrary values of N. The figure shows the positions for time $t = 0$, with angles given by $\varphi_i = (i-1)2\pi/N$. (1 point)

b) Calculate (analytically) the total force $\vec{F}_1$ acting on body 1 at time $t = 0$. This gives

$$\vec{F}_1 = \begin{pmatrix} F_x \\ 0 \end{pmatrix}, \quad \text{mit} \quad F_x = -\frac{Gm^2}{4R^2} \sum_{j=2}^{N} \frac{1}{\sin((j-1)\frac{\pi}{N})} \, .$$

(3 points)

c) From Newton's equation of motion, calculate the velocity v of the bodies. This results in:

$$v^2 = \frac{Gm}{4R} \sum_{j=2}^{N} \frac{1}{\sin((j-1)\frac{\pi}{N})} \ . \tag{1}$$

(1 point)

d) Write a code which simulates the movement of the N bodies via a numerical solution of the set of couples differential equations. Show that with the velocities given in eq. (1), the bodies indeed perform circular orbits as in part a). (6 points)

e) Check whether these orbits are stable or unstable with respect to small changes in the initial conditions, such as displacing one of the bodies at time $t = 0$ by a small amount. (2 points)