M2 PTSC et MSA
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Simulation numérique en physique statistique
TD n° 6

Advanced Monte Carlo Methods

1 Wang Landau method

The algorithm developed by Wang and Landau is a method able to compute the density of states in energy $g(E)$ in a bounded interval of energy.

▷ **1-1** Using detailed balance, re-derive the form of the transition rate for going from a configuration of energy E into one of energy E' which is at the basis of this algorithm. Explain how the energy histogram should be modified after each change of configuration.

▷ **1-2** Why is it needed to reduce the modification factor after each iteration in the algorithm ? Why is it needed to also reset the histogram after each iteration ?

▷ **1-3** At the start of the simulation, the density of state is generally assumed to be constant and equal to one. What would be happen if one were to start from a different initial condition ?

▷ **1-4** The Wang Landau algorithm is usually implemented using local moves of the type used in the Metropolis algorithm. When the dynamics involves many particles why does the efficiency of the Metropolis algorithm decreases with system size and not that of the Wang Landau algorithm ?

▷ **1-5** Near a first order transition, the canonical distribution has generally a double peak structure. Draw the general shape of this distribution when going from $T < T_c$ to $T > T_c$. How is this picture modified when the size of the system increase ?

▷ **1-6** Why is conventional Monte Carlo simulation not particularly efficient in this case and how does the Wang Landau algorithm overcome this problem ?

2 Dynamic Monte Carlo

Dynamic simulations of the Ising model using the Metropolis algorithm are not particularly efficient at low temperatures due to rejections. To overcome this problem, one may attempt to construct a Markov chain between accepted configurations rather than attempted configuration. Such a method was devised by Bortz, Kalos and Lebowitz in 1975, and is known under the name of "N-fold way" or "Faster than the clock algorithm".

▷ **2-1** In the 2D Ising model, containing N spins, what is the probability of flipping one arbitrary spin according to the Metropolis rule ?

▷ **2-2** What is the probability that no spin has occurred anywhere in the lattice ?

▷ **2-3** Using a random number, explain how to calculate numerically the average time to the next spin flip ?

▷ **2-4** The various environments experienced by a given spin the lattice fall into different classes, where each class is defined by the number of up and down neighboring spins. How many classes exist for a spin in the 2D Ising model with periodic boundary conditions ? Note that a spin flip produces changes of classes in neighboring spins.

▷ **2-5** Explain how to construct an efficient algorithm based on only moves between accepted configurations among classes. [See related short programs on website to apply these ideas.]