Physics of Complex Systems

Université Pierre et Marie Curie (Paris VI)

Advanced simulation techniques and mathematical tools

(18 December 2013 - duration: 3h)

The exam consists of three independent parts. The questions of each part are also independent and can be solved by using previous results. It is not necessary to answer all questions to obtain full credit.

Lecture notes are allowed.

1 Zero range process

One considers a model in which N undistinguishable particles occupy sites of a one dimensional lattice of L sites labelled from 1 to L. Each site of the lattice contains one or several particules. Dynamics of the system is a stochastic process where a particle of site i can hop on the site $i+1$ with a rate $u(n_i)$ which only depends on the particle number n_i of the site of departure. Periodic boundary conditions are applied, which means that a particle on the site L hops on the site 1.

▷ **1-1** One first assumes that $u(n)$ is independent of n for $n > 0$ and $u(0) = 0$. One considers a Monte Carlo algorithm in which a site is uniformly selected at each time step and a particle is moved if the site is not empty. Justify that the transition matrix element of the Monte Carlo dynamics of changing the state of the site i is given by

$$w(n_i \to n_i + 1) = \frac{1}{L} \frac{u(n_i)}{\sum_{i=1}^{L} u(n_i)} \tag{1}$$

▷ **1-2** To increase the efficiency of the algorithm, one only selects randomly an occupied site. Show that this algorithm leads to the same stationary state

▷ **1-3** When $u(n) = n$, justify that the Monte Carlo algorithm can be modified by choosing randomly a particle at each time step instead of a site.

▷ **1-4** The probability of having a configuration is defined as $p(\{n_\mu\})$ where $\{n_\mu\}$ is a set of particle number with $\mu \in [1, n]$. Show that the stationnary state of the master equation describing the Monte Carlo algorithm is given by

$$\sum_{\mu=1}^{L} u(n_{\mu-1} + 1)p(..., n_{\mu-1} + 1, n_\mu - 1, ...) - u(n_\mu)p(\{n_\mu\})\theta(n_\mu) = 0 \tag{2}$$

where θ is a Heaviside function.

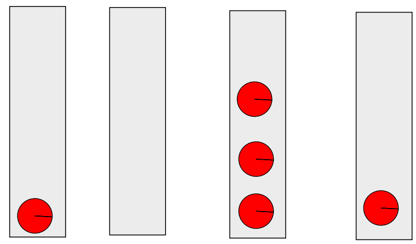

Figure 1: Configuration of Zero range model

▷ **1-5** Show that the detailed balance does not hold.

The steady probability can be written as $p(\{n_\mu\} = \frac{1}{Z_{N,L}} \prod_{\mu=1}^{L} f(n_\mu)$ where $f(n)$ is a scalar factor.

▷ **1-6** Show that

$$u(n_{\mu-1}+1)f(n_{\mu-1}+1)f(n_\mu - 1) = u(n_\mu)f(n_{\mu-1})f(n_\mu) \tag{3}$$

▷ **1-7** Infer that

$$u(n_\mu)\frac{f(n_\mu)}{f(n_\mu - 1)} = C \tag{4}$$

where C is a constant.

▷ **1-8** Without loss of generality, we set $C = 1$. Show that $f(n)$ can be expressed as a product of $u(i)$ with $i \in [1, n]$ for $n > 0$ and $f(0) = 1$.

▷ **1-9** Show that the normalization $Z(L, N)$ is given by

$$Z(L, N) = \sum_{\{n_\mu\}} \prod_{\mu=1}^{L} f(n_i)\delta(\sum_{\mu=1} n_\mu - N) \tag{5}$$

where δ is the Kronecker symbol.

One considers a one-to-one mapping of the zero-range process with the following model: A vacant site of the zero range model is replaced with an occupied site with one particle; an occupied site of the zero range model with n particles is replaced with a sequence of $n+1$ sites with a first site is occupied with one particle and the other n vacant sites .

▷ **1-10** Consider the configuration of the zero range model (Fig. 1) and draw the corresponding configuration of the other model

▷ **1-11** For a zero range model with L sites and N particles, how many sites do we need in the other model?

▷ **1-12** When $u(n) = 1$ for $n > 0$, $u(0) = 0$, justify that the other model corresponds to a totally exclusion process; in particular, show that a site can be occupied by two particles.

2 Ergocity of the Nosé-Hoover algorithm

We illustrate here that the Nose-Hoover algorithm does provide an erdogic algorithm for sampling a canonical ensemble. We start by non-Hamiltonian equations of motion (the equations are different from those given in the lecture notes, but we can show that there are equivalent).

Consider a system of N interacting point particles; the potential is $\phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$. The force acting on particle i is $\mathbf{F}_i = -\boldsymbol{\nabla}_{\mathbf{r}_i}\phi$. The equations of motion are given by

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i}, \qquad \dot{\mathbf{p}}_i = \mathbf{F}_i - \frac{p_\eta}{Q}\mathbf{p}_i$$

$$\dot{\eta} = \frac{p_\eta}{Q}, \qquad \dot{p}_\eta = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{m_i} - Lk_B T\eta \tag{6}$$

where $\mathbf{r}_i$, m_i and $\mathbf{p}_i$ are the position, the mass and the momentum of the particle i respectively; η, Q and p_η are the position, the mass and the momentum of the fictive particle; k_b the Boltzmann constant,T the temperature and L an integer to be determined.

▷ **2-1** Show that the "total" energy H' is a conversed quantity where

$$\begin{aligned} H' &= \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m_i} + \phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) + \frac{p_\eta^2}{2Q} + Lk_B T\eta \\ &= H(\mathbf{r}^N, \mathbf{p}^N) + \frac{p_\eta^2}{2Q} + Lk_B T \end{aligned} \tag{7}$$

One assumes that H' is the only conversed quantity. The microcanonical partition function $Z(N, V, E_1)$ of the entire system reads

$$Z(N, V, E_1) = \int d\mathbf{p}^N \int d\mathbf{r}^N \int dp_\eta \int d\eta e^{dN\eta} \delta(H' - E_1) \tag{8}$$

where d is the space dimension.

▷ **2-2** Integrate over η and p_η and show that the result is proportional to the canonical partition $Q(N, V, T)$ for a value of L to be determined.

▷ **2-3** However, additional conserved quantities can be obtained. Noting that no external force is applied to the system and by using the equations of motion show that $\mathbf{P}e^\eta$ is a constant vector with $\mathbf{P} = \sum_{i=1}^{N} \mathbf{p}_i$.

Show that the change of variable $\mathbf{p}_i = m_i\mathbf{v}_i$ with $i \in [1, N]$ and $\mathbf{p}'_i = m_i\mathbf{v}'{}_i, \mathbf{P}$ with $i \in [1, N-1]$ and $\mathbf{v}'_i = \mathbf{v}_i - \mathbf{V}$, is a canonical transformation, namely the Jacobian of the transformation is equal to 1.

▷ **2-4** Show that the kinetic energy E_c of the N-particle system is now given by

$$E_c = \sum_{i=1}^{N-1} \frac{\mathbf{p}'^2_i}{2m_i} + \frac{(\sum_{i=1}^{N-1} \mathbf{p}')^2}{2m_n} + \frac{P^2}{2M} \tag{9}$$

where $M = \sum_{i=1}^{N} m_i$.

▷ **2-5** Introducing $\mathbf{r'}_i = \mathbf{r}_i - \mathbf{R}$, with $\mathbf{R}$ the position of the center of mass, show that the equations de motion are now given by

$$\dot{\mathbf{r}'}_i = \frac{\mathbf{p'}_i}{m_i}, \qquad \dot{\mathbf{p}'}_i = \mathbf{F}_i - \frac{p_\eta}{Q}\mathbf{p'}_i, \qquad \dot{P} = -\frac{p_\eta}{Q}P$$
$$\dot{\eta} = \frac{p_\eta}{Q}, \qquad \dot{p}_\eta = 2E_c - Lk_BT \tag{10}$$

The correct partition function must include all conservation laws. Consequently, this gives

$$Z(N,V,E_1,K) = \int\cdots\int d^{N-1}\mathbf{p'}dPd^{N-1}\mathbf{r'}dp_\eta d\eta e^{(d(N-1)+1)\eta}\delta(H(\mathbf{p'},\mathbf{r'}) + \frac{p_\eta^2}{2Q} + LkT\eta - E_1)\delta(e^\eta P - K) \tag{11}$$

▷ **2-6** Integrate over η, and over p_η and show that

$$Z(N,V,E_1,K) \propto \int d^{N-1}\mathbf{p'}dP\int d^{N-1}\mathbf{r'}\left(\frac{K}{P}\right)^{(d(N-1)+1)}\frac{1}{\sqrt{E_1 - H(\mathbf{p'},\mathbf{r'}) - Lk_BT\ln(K/P)}} \tag{12}$$

▷ **2-7** For a free particle in one dimension, show that the distribution velocity is given by

$$f(p,E_1,K) \propto \frac{1}{\sqrt{p^2(K - (p^2/2m) + Lk_BT\ln(p/K))}} \tag{13}$$

▷ **2-8** By studying the variation of the denominator show that the velocity distribution is only defined in a finite interval of momentum.

3 Detailed Jarzynski equality for a logically irreversible procedure

We consider a system obeying a stochastic dynamics with a Hamiltonian $H(x,\lambda)$, where x is the fluctuating variable which is observed and λ is a variable which is controlled externally. The system is in contact with a heat bath at the temperature $T = 1/\beta$. In the absence of non-conservative forces, the expression of the work in a process that starts at x_0 at time 0 with a value of the control parameter fixed to λ_0 and ends at position $x(t) = x_t$ at time t with $\lambda(t) = \lambda_t$ is

$$W = \int_0^t dt'\dot{\lambda}_t\frac{\partial H(x_t,\lambda_t)}{\partial\lambda}. \tag{14}$$

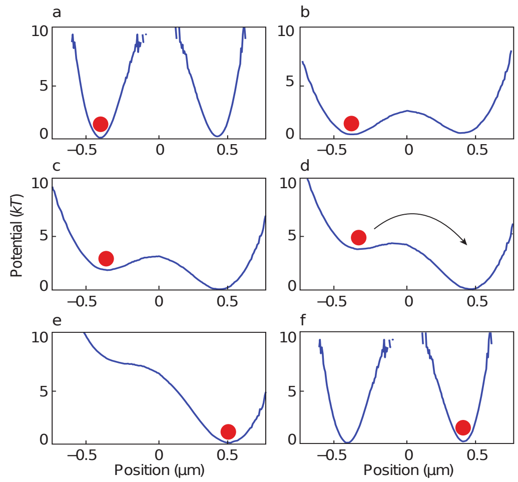

Figure 2: Evolution of the potential in chronological order from state a to state f when a time-dependent force is applied to a brownian particle represented here as the red circle.

We now assume that the system starts initially at $t = 0$ at equilibrium, characterized by a p.d.f. $\rho_{eq}(x, \lambda)$ and ends at time t in a non-equilibrium state characterized by a p.d.f. $\rho(x, t)$. It is possible to prove a variant of Jarzynski relation in the form

$$\langle \delta(x - x_t) e^{-\beta W} \rangle = \frac{e^{-\beta H(x,\lambda_t)}}{Z_0}, \tag{15}$$

where Z_0 represents the partition function at the initial state.

▷ **3-1** Derive from this equation the relation which is usually known as the Jarzynski relation.

▷ **3-2** Show that Eq. 15 is equivalent to

$$\frac{\rho(x, t)}{\rho_{eq}(x, \lambda_t)} \langle e^{-\beta W} | x = x_t \rangle = e^{-\beta \Delta F(t)}, \tag{16}$$

where the notation $\langle .. | x = x_t \rangle$ means a conditional average for the variable x_t to have the value x at time t and $\Delta F(t)$ is a quantity which you will define.

We now want to apply these results to an experiment which consists in manipulating a brownian particle by applying a time-dependent force with a given protocol (see Fig.2). Initially, the particle is in a symmetric potential and it can be found in one of the two wells of the potential with equal probability (Fig 2a). Then the barrier of this potential is lowered (Fig 2b), it is tilted (Fig 2c,d) in such a way that the particle always ends up in the right minimum of the potential (Fig 2e). The force is then returned to its original value (Fig 2f).

▷ **3-3** What are the difference of free energy and internal energy during a complete cycle of such a process, why ?

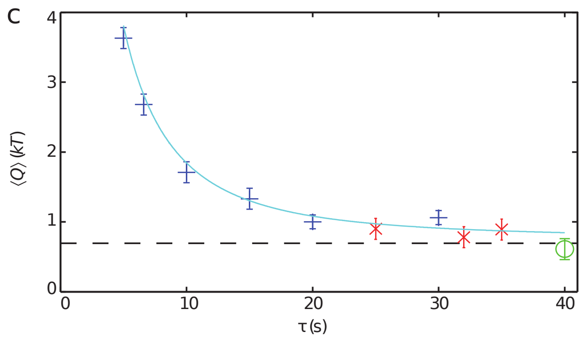

Figure 3: Evolution of the average heat divided by k_BT as a function of the duration of the cycle τ. The symbols represent experimental data points. Evolution de la chaleur moyenne divisée par k_BT comme une fonction de la durée du cycle τ. Les symboles réprésentent les points expérimentaux.

▷ **3-4** Show that in these conditions,

$$\langle e^{-\beta W} \rangle_{\to 0} = \frac{1}{2}, \tag{17}$$

where the notation $\langle .. \rangle_{\to 0}$ means an average over a process which will end with the particle in the right minimum of the potential as in figure 2f.

▷ **3-5** We now assume that the process is not perfect and that the particle ends up most of the time in the right minimum (with probability P_s), but occasionnaly may also end up in the left minimum (with probability $1 - P_s$). Calculate the corresponding exponential average of the work for these two situations and show that together they are compatible with the Jarzynski relation.

▷ **3-6** From the results obtained above, derive a bound for the average work which depends only on P_s (irrespectively of the final state). Show that this bound can be interpreted as a change of entropy of the system.

▷ **3-7** Fig. 3 shows the average heat recorded in the experiment as function of the duration of the cycle. Explain how this experiment relates with the Landauer principle which states that in any irreversible logical operation, the minimum dissipation is $-k_B \ln(2)$ per bit involved in the logical operation.