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Comparison of Langevin and Monte Carlo dynamics

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Abstract. The Monte Carlo and Langevin dynamical methods of simulating the thermodynamics of physical systems are compared by calculating relaxation times according to the two dynamics for a system which is analytically tractable, namely a single (planar) spin in a potential which has either a single minimum or two minima separated by a barrier. With no restriction on the maximum allowed spin reorientation per Monte Carlo step the Langevin method is faster than the Monte Carlo method for the single minimum potential. However a careful choice of restriction can make the Monte Carlo method as efficient as the Langevin method. For the double-well potential the Monte Carlo method with no restriction is the most efficient. One is forced to use a finite-time step size when numerically solving the Langevin equation and the departures this produces from the equilibrium Boltzmann distribution are studied.

1. Introduction

In recent years, computer simulation has provided physicists with a large amount of valuable information, especially in the field of statistical physics where exact solutions can only be found for a small number of systems. Most of these simulations are based on the Monte Carlo method. This involves setting up a Markovian process in which the state of a system is iteratively replaced by a new configuration at each step. The transition probabilities from one state to another are chosen in such a way that the process will give the canonical (Boltzmann) equilibrium distribution. Free energies and other static thermodynamical quantities can be obtained by averaging these variables over many steps (Muller-Krumbhaar and Binder 1973).

The Monte Carlo method is by no means the only one used to simulate a statistical system. Other methods such as solution of the Langevin equation have also been suggested and used, both in the field of statistical physics (Bray and Moore 1982, Meakin *et al* 1983) and in the field of particle physics (Parisi 1980, 1981, Drummond *et al* 1982, Thomas 1984). The important point about these methods is that they all, in principle, have the same equilibrium distribution, namely the Boltzmann distribution, so any of them can be used as far as the computation of static thermodynamic variables is concerned. However, one must note that in order to eliminate the effects of the initial conditions, one needs to let the simulated system relax into equilibrium before the process of averaging is started. In other words, the first M steps must be omitted from the averaging. M is such that it should always be greater than τ_r/τ_s , where τ_r is the longest relaxation time of the system and τ_s is the step time (the time between two steps). Obviously, the method which provides the smallest relaxation time per step time is more efficient in the sense that fewer steps are omitted and hence less

computational time is wasted. Also the statistical error on the result obtained from a simulation is of order \sqrt{M}/\sqrt{N} where N is the number of steps included in the averaging. Hence, in this respect the method with a smaller M (relaxation time per step time) can also be considered more efficient as it provides results with a higher accuracy for the same number of steps N .

In the first part of this paper we have compared the Monte Carlo dynamic, governed by the master equation (Muller-Krumbhaar and Binder 1973), to the Langevin dynamic by calculating the relaxation times at low temperatures. In order to do so we first had to define the step time τ_s for the Monte Carlo case. This is chosen in such a way as to make the relaxation times of both dynamics equal in the high-temperature limit. In fact, the choice of τ_s does not affect the equilibrium distribution in the case of the Monte Carlo method. It simply defines the time scale for the process (Binder 1979). However, in the case of the Langevin method this is not so. As stated before both of the methods have the Boltzmann distribution as their steady state solutions. This is true in principle. But one must realise that when one is trying to solve a differential equation such as the Langevin equation on a computer, the differential equation has to be replaced by a recurrence relation. In other words, one replaces dx/dt by $\Delta x/\Delta t$ where Δt has a finite value. In doing so, a certain degree of error is introduced and instead of the Boltzmann distribution one gets a slightly different distribution as the steady state solution. The error is proportional to Δt (Parisi 1980). Here, Δt is just the step time τ_s . Thus the amount of error which can be tolerated puts an upper limit on the size of the step time. This effect will be discussed in some detail in § 5.

The calculations are performed for a single classical planar spin moving in (1) a potential $-h \cos \theta$ and (2) a potential $D \sin^2 \theta$. The first potential is a single-well potential and represents the coupling between the spin and a magnetic field. The second case is a double-well potential and can be regarded as an anisotropy field. It is found that the Langevin equation approach is superior in the first case. However, one can increase the efficiency of the Monte Carlo method by restricting the maximum allowed change in the angle at each step. The choice of maximum allowed change in the angle is critical and strongly affects the relaxation time. It is shown that with a good choice one can make the Monte Carlo method as efficient as the Langevin equation approach. In the second case, where a potential barrier separates two equilibrium spin orientations, the Monte Carlo method is the better of the two. In this case the greatest efficiency is obtained when no restrictions are imposed on the maximum allowed change in the angle. The result is intuitively obvious. Because the calculations of the various relaxation times in the two dynamics can be performed analytically for this very simple system, we can for once establish quantitatively the superiority of one dynamic over another. Moreover we expect that the features revealed by these calculations will be true of more complex systems, such as interacting spins, where direct analytic calculations of the kind performed here will not be feasible.

We have to point out that in certain special cases, for example when calculating the connected correlation functions in the regions where they are small, it is still advantageous to use the Langevin dynamic method (Parisi 1980, 1981). In some cases the Langevin method might even be the only reasonable method that one can use. For example if one is interested in *dynamical* processes themselves, as represented by time-dependent correlation functions, then one simply has to use the appropriate dynamical equations. For non-Ising spins, e.g. planar or Heisenberg spins, the Monte Carlo method never provides realistic dynamical equations. However, in certain situations, the Langevin equation may be realistic (Beton and Moore 1984).

In § 2, we describe our simple model in some detail and specify the two dynamics. In § 3 we obtain the low-temperature behaviour according to the two dynamics for the single-well potential and discuss the effect of restricting the change in the angle for the Monte Carlo case. In § 4 we repeat the process for the double-well potential.

2. Models and dynamics

We shall consider a single planar spin of unit length governed by either the ‘magnetic field’ Hamiltonian

$$\mathcal{H}(\theta) = -h \cos \theta, \tag{1}$$

or the ‘anisotropy’ Hamiltonian

$$\mathcal{H}(\theta) = D \sin^2 \theta. \tag{2}$$

In (1), θ is the angle between the direction of the field and that of the spin, and $0 \leq \theta \leq 2\pi$. There is one ‘easy’ direction of the spin along $\theta = 0$, i.e. the potential has a single well. The double-well potential (2) is typical of uniaxial anisotropy and the easy directions are $\theta = 0$ and $\theta = \pi$.

The Langevin equation for a planar spin is of the form

$$d\theta/dt = -\partial\mathcal{H}/\partial\theta + f(t), \tag{3}$$

where $f(t)$ is a white-noise source generated by the coupling of the spin to its surroundings (a ‘heat bath’) with strength

$$\langle f(t)f(t') \rangle = 2k_B T \delta(t - t'). \tag{4}$$

Using equation (3) one can derive an equation for the probability distribution $P(\theta, t)$. This is just the Fokker–Planck equation (Chandrasekhar 1943, Wang and Uhlenbeck 1945), the eigenvalues of which would give us the relaxation times. The Fokker–Planck equation for a planar spin has the form

$$k_B T \partial^2 P / \partial \theta^2 + (\partial \mathcal{H} / \partial \theta) \partial P / \partial \theta + (\partial^2 \mathcal{H} / \partial \theta^2) P = \partial P / \partial t. \tag{5}$$

It is easily seen that the equation has the Boltzmann distribution $\exp(-\beta H)$ as its steady state solution as expected.

The Monte Carlo dynamic is described by the master equation (Muller-Krumbhaar and Binder 1973)

$$\frac{\partial P(\theta, t)}{\partial t} = \int \omega(\theta', \theta) P(\theta', t) d\theta' - \int \omega(\theta, \theta') P(\theta, t) d\theta'. \tag{6}$$

$\omega(\theta, \theta')$ specifies the transition rate from a state θ to a state θ' and from now on we will take it as being that specified by the Metropolis algorithm (Metropolis *et al* 1953). That is

$$\omega(\theta, \theta') = \begin{cases} (2\pi\tau_s)^{-1} & \delta\mathcal{H} < 0 \\ (2\pi\tau_s)^{-1} \exp(-\delta\mathcal{H}/k_B T) & \delta\mathcal{H} > 0. \end{cases} \tag{7}$$

This choice is made because the Metropolis (1953) algorithm is particularly simple to use on a computer and hence is the one most frequently used in numerical work. τ_s appearing in (7) is the step time, in other words τ_s^{-1} transitions are performed within the unit time.

In § 3 we shall solve equations (5) and (6) for the case of a single-well potential and compare the results.

3. The solutions of the Langevin and master equations for the case of the single-well potential

With a potential described by (1), the Fokker-Planck equation (5) becomes

$$k_B T \partial^2 P / \partial \theta^2 + h \sin \theta \partial P / \partial \theta + h \cos \theta P = \partial P / \partial t. \quad (8)$$

In the high-temperature limit, $h \ll k_B T$, one expects the behaviour of the system to be similar to that of a free spin with no magnetic field present. For this limit one can approximate equation (8) by

$$k_B T \partial^2 P / \partial \theta^2 = \partial P / \partial t \quad (9)$$

which can easily be solved to give

$$P(\theta, t) = \sum_{\lambda \geq 0} [A_\lambda \sin(\lambda/k_B T)^{1/2} \theta + B_\lambda \cos(\lambda/k_B T)^{1/2} \theta] e^{-\lambda t}.$$

The periodic boundary conditions $P(\theta, t) = P(\theta + 2\pi, t)$ restricts the values of λ to $n^2 k_B T$, where n is an integer. It follows that the dominant (i.e. slowest) relaxation time is $1/k_B T$ and the steady state solution is a uniform distribution as expected for the high-temperature limit. The equation can also be solved in the low-temperature limit if one realises that in this limit, $h \gg k_B T$, the spin will nearly always be parallel to the field. That is, the probability of having a large θ is very small. Using this fact we can approximate the potential by

$$\mathcal{H}(\theta) = -h \cos \theta \approx -h(1 - \frac{1}{2}\theta^2)$$

which leads to the following Fokker-Planck equation

$$k_B T \partial^2 P / \partial \theta^2 + h\theta \partial P / \partial \theta + hP = \partial P / \partial t \quad (10)$$

which now has to satisfy the boundary condition $P(\theta, t) \rightarrow 0$ as $\theta \rightarrow \infty$. The solution to equation (10) is of the form

$$P(\theta, t) = \sum_{\lambda \geq 0} f_\lambda(\theta) e^{-\lambda t}$$

where $f(\theta)$ has to satisfy

$$\partial^2 f / \partial \theta^2 + (h\theta/k_B T) \partial f / \partial \theta + [(h + \lambda)/k_B T] f = 0.$$

Using the transformations

$$f(\theta) = \phi(\theta) \exp(-h\theta^2/2k_B T)$$

followed by

$$\theta = (2k_B T/h)^{1/2} x$$

the equation can be transformed into Hermite's equation

$$\partial^2 \phi / \partial x^2 - 2x \partial \phi / \partial x + (2\lambda/h) \phi = 0$$

which together with the boundary condition stated above restricts the eigenvalues to

$$\lambda = nh \quad n = 0, 1, 2, \dots$$

with corresponding eigenfunction

$$\phi(x) = H_n(x)$$

where $H_n(x)$ is the n th Hermite polynomial. Thus the solution to equation (10) becomes

$$P(\theta, t) = \sum_{n=0}^{\infty} \alpha_n H_n((h/2k_B T)^{1/2} \theta) \exp(-h\theta^2/2k_B T) \exp(-nht) \quad (11)$$

with a dominant relaxation time $1/h$ which, unlike the high-temperature limit, is independent of T .

These results must be compared to the solutions of the master equation (6) in the same temperature limits. With a Hamiltonian described by (1) the transition probabilities (7) will become

$$\omega(\theta, \theta') = \begin{cases} (2\pi\tau_s)^{-1} & |\theta'| < |\theta| \\ (2\pi\tau_s)^{-1} \exp[\beta h(\cos \theta' - \cos \theta)] & |\theta'| > |\theta| \end{cases} \quad (12)$$

where $\beta = 1/k_B T$. Substituting (12) into (6) gives

$$\begin{aligned} \frac{\partial P(\theta, t)}{\partial t} = & -P(\theta, t) \left(\int_{-|\theta|}^{+|\theta|} (2\pi\tau_s)^{-1} d\theta' + \int_{-\pi}^{-|\theta|} (2\pi\tau_s)^{-1} \exp[\beta h(\cos \theta' - \cos \theta)] d\theta' \right. \\ & + \int_{+|\theta|}^{\pi} (2\pi\tau_s)^{-1} \exp[\beta h(\cos \theta' - \cos \theta)] d\theta' \left. \right) \\ & + \int_{-|\theta|}^{+|\theta|} (2\pi\tau_s)^{-1} P(\theta', t) \exp[\beta h(\cos \theta - \cos \theta')] d\theta' \\ & + \int_{-\pi}^{-|\theta|} P(\theta', t) (2\pi\tau_s)^{-1} d\theta' + \int_{+|\theta|}^{\pi} P(\theta', t) (2\pi\tau_s)^{-1} d\theta'. \end{aligned} \quad (13)$$

The equation takes a relatively simple form in the high-temperature limit $h \ll k_B T$, since in this limit all the terms $\exp[\beta h(\cos \theta' - \cos \theta)]$ tend to unity independently of the values of θ and θ' and we get

$$\begin{aligned} \frac{\partial P(\theta, t)}{\partial t} = & \int_{-\pi}^{+\pi} P(\theta', t) (2\pi\tau_s)^{-1} d\theta' - P(\theta, t) \tau_s^{-1} \\ = & -P(\theta, t) \tau_s^{-1} + (2\pi\tau_s)^{-1} \end{aligned}$$

which can easily be solved:

$$P(\theta, t) = (2\pi)^{-1} + A(\theta) \exp(-t\tau_s^{-1}). \quad (14)$$

$A(\theta)$ is a periodic function of θ determined by the initial conditions. From the above solution it can be seen that the steady state distribution is uniform as one expects, and the relaxation time is equal to the step time τ_s . As mentioned earlier, the value of τ_s does not affect the equilibrium distribution in the case of the Monte Carlo simulation. Hence by taking $\tau_s = 1/k_B T$, we can make the Langevin and the Monte Carlo dynamic consistent in the high-temperature limit. In this way we have also defined the time scale for the Monte Carlo method.

We have not been able to solve the master equation (13) directly in the low-temperature limit. However, a lower bound for the dominant relaxation time has been found using a variational method. To see how this can be done one writes equation (13) in the alternative form:

$$\frac{\partial P(\theta, t)}{\partial t} = \int_{-\pi}^{+\pi} \left(\min((2\pi\tau_s)^{-1}, \exp[\beta h(\cos \theta - \cos \theta')](2\pi\tau_s)^{-1}) - \delta(\theta - \theta') \int_{-\pi}^{+\pi} \min((2\pi\tau_s)^{-1}, \exp[\beta h(\cos \theta'' - \cos \theta)] \times (2\pi\tau_s)^{-1}) d\theta'' \right) P(\theta', t) d\theta'.$$

Substituting a solution of the form $f_\lambda(\theta) e^{-\lambda t}$ into the above equation gives the integral equation

$$-\lambda f_\lambda(\theta) = \int_{-\pi}^{+\pi} k(\theta, \theta') f_\lambda(\theta') d\theta' \tag{15}$$

with a kernel

$$k(\theta, \theta') = \min((2\pi\tau_s)^{-1}, \exp[\beta h(\cos \theta - \cos \theta')](2\pi\tau_s)^{-1}) - \delta(\theta - \theta') \int_{-\pi}^{+\pi} \min((2\pi\tau_s)^{-1}, \exp[\beta h(\cos \theta'' - \cos \theta)](2\pi\tau_s)^{-1}) d\theta''. \tag{16}$$

The first eigenstate of equation (15) is already known since it is just the steady state solution with $\lambda = 0$. The eigenfunction has the Boltzmann distribution form:

$$f_0(\theta) = \exp(h \cos \theta / k_B T).$$

If one could find a function which when multiplied into equation (15) puts it into a form where the kernel is symmetric in θ and θ' , then according to the Hilbert-Schmidt theory (Courant and Hilbert 1953), one knows that any two different eigenfunctions of this new equation are orthogonal and they form a complete set. Thus, it is possible to carry out a variational calculation for the second eigenvalue.

The details of this calculation are given in appendix 1 and it is shown that in the low-temperature limit, ($h \gg k_B T$), the second eigenvalue is such that

$$\lambda \leq 3\tau_s^{-1} (2k_B T / \pi^3 h)^{1/2}.$$

With $\tau_s = 1/k_B T$ as before, the dominant relaxation time τ_r becomes

$$\tau_r = \lambda^{-1} \geq \frac{1}{3} h^{1/2} \pi^{3/2} 2^{-1/2} (k_B T)^{-3/2}. \tag{17}$$

Thus, comparing this result with that obtained for the Langevin method ($\tau_r = 1/h$), it can be seen that in the low-temperature limit the Monte Carlo method specified by transition probabilities (12) (which imply *no* restriction on the maximum value of change in the angle in one step) is slower than Langevin dynamics for a single-well potential. In order to improve the Monte Carlo method, transition probabilities (12) have to be modified in such a way that they will limit the change in the angle to a certain value. For the best result this value must be chosen carefully to be a specific function of temperature. We argue below that Δ , the limit on the maximum change

in the angle, has to be proportional to $T^{1/2}$ if the smallest relaxation time is to be obtained.

At first sight it might seem that the restriction imposed on the change in the angle will limit movement in phase space and thus would increase the relaxation time. However, this is not the case. Consider a spin in a state close to the bottom of the well and at low temperatures. The range of angles for which the energy would decrease would be a rather small proportion of the total angles which could be chosen for the next step if there is no restriction. This means the chance of accepting a move would be small and the system would remain in the same state for a large number of steps. This gives rise to a long relaxation time. Now, if one restricts the magnitude of change in the angle to be smaller than Δ , then the angles for which the energy would decrease will be a much larger proportion of the total angles which can be picked for the next step and should improve the relaxation time. A good value for Δ has to ensure that on average the chance of accepting a move at each step has to be about half, but at the same time it must not be so small as to restrict the movement in phase space unnecessarily. From equipartition, the average magnitude of the angle θ at low temperatures is approximately proportional to $T^{1/2}$. If Δ is approximately T^n for $n < \frac{1}{2}$ the value of Δ will be much larger than the average magnitude of θ at low temperatures. In this case one expects the results to be similar to those of the case with no restriction. On the other hand, if one chooses $n > \frac{1}{2}$ then Δ will be much smaller than the average value of θ as temperature decreases, and this produces severe restriction on the movement in phase space which will give rise to a long relaxation time. Thus it follows that the best value for n should be $\frac{1}{2}$. This ensures that the ratio of the average value of θ (or more precisely RMS value of θ) to Δ stays constant as temperature is varied. Choosing $\Delta \approx (\beta h)^{-1/2}$ the transition probabilities can be written as

$$\omega(\theta, \theta') = \begin{cases} = 0 & |\theta - \theta'| > \Delta \\ = (2\Delta\tau_s)^{-1} & |\theta - \theta'| < \Delta, \delta\mathcal{H} < 0 \\ = (2\Delta\tau_s)^{-1} \exp[\beta h(\cos \theta' - \cos \theta)] & |\theta - \theta'| < \Delta, \delta\mathcal{H} > 0. \end{cases}$$

Carrying out a variational calculation similar to that already performed for the case with no restriction, gives a lower bound for the relaxation time $\approx \tau_s = 1/k_B T$. Although this result and the result (17) are both only lower bounds, we expect the actual relaxation times to have the same temperature dependence. Comparing the two Monte Carlo methods one can see that the relaxation time at the low-temperature limit has improved by imposing a restriction on the value of the maximum allowed change in the angle that can take place in one step. However, it is still longer than the relaxation time for the Langevin method. At first this might suggest that the Langevin method is more efficient than the Monte Carlo case. However, the efficiency of the method is not determined only by its relaxation time but also by the step time, in other words it is determined by τ_t/τ_s . As will be seen later it follows that the Monte Carlo method with the restriction can be made as efficient as the Langevin method.

4. The case of a double-well potential

The results obtained in § 3 might not be true in general if one is dealing with potentials more complicated than that given by (1). To see why this might be so, consider a double-well potential such as that described by (2). The important difference between this and a single-well potential such as (1) is the presence of a barrier in (2). This

means that in the case of the Langevin method, the spin needs to gain sufficient energy from its surroundings in order to make a transition from one well into the other. The white noise $f(t)$, representing the interaction of spin with its surroundings in equation (3), has a strength which decreases as temperature is decreased. Therefore, the probability of obtaining sufficient energy to overcome the barrier becomes very small at low temperatures and large barrier heights, which leads to very long relaxation times as compared to the relaxation times for a single-well potential.

Unlike the Langevin method, the relaxation times for a single and double-well potential are not expected to be very different in the case of the Monte Carlo method with no restriction. If the spin is in a state θ and a new state θ' is chosen in the next step, a transition from θ to θ' is definitely made if that involves a decrease in energy, otherwise, it is made with a probability $\exp(-\beta\delta E)$. This is true whether θ and θ' are states within the same well or within different ones. Thus, even at low temperatures and large barrier heights, transitions from one well into another can easily take place.

We shall support the above view by calculating the relaxation times for both dynamics. The Monte Carlo method with restriction is not discussed as it is unlikely that this improves the efficiency of the method as far as potentials with barriers in them are concerned.

Substituting (2) into the Fokker-Planck equation (5), we obtain

$$\partial P/\partial t = k_B T \partial^2 P/\partial \theta^2 + D \sin 2\theta \partial P/\partial \theta + (2D \cos 2\theta) P. \quad (18)$$

At this stage one can use Kramer's method (Chandrasekhar 1943) to calculate the relaxation time. This method is based on the assumption that the equilibrium is established much faster within the individual wells compared to the time taken for it to be established between the two wells. Kumar and Dattagupta (1983) have presented an argument justifying the above view. Brown (1963) has obtained the relaxation time for the more complicated case of a Heisenberg spin in a double-well potential. Our calculations are very similar to those of Brown and for that reason we shall omit the detail and simply quote the answer. The largest eigenvalue determining the dominant relaxation time is given by

$$\lambda = 2/(\beta I_m)^{-1}(I_1^{-1} + I_2^{-1}) \quad (19)$$

where

$$I_m = \exp(\beta V(\pi/2))(2\pi)^{1/2}(\beta V''(\pi/2))^{-1/2} \quad (20a)$$

$$I_1 = (2\pi/\beta V''(0))^{1/2} \exp(-\beta V(0)) \quad (20b)$$

$$I_2 = (2\pi/\beta V''(\pi))^{1/2} \exp(-\beta V(\pi)). \quad (20c)$$

Using potential (2) and results (19)-(20), we have a relaxation time

$$\tau_r = \lambda^{-1} \sim \exp(\beta D). \quad (21)$$

One can also get an estimate of the relaxation time for the Monte Carlo case with potential (2). The calculations are given in appendix 2 and show that the relaxation time required for the equilibrium to be achieved between two wells is

$$\tau_r \approx \frac{1}{8}(\pi\beta D)^{1/2} \tau_s. \quad (22)$$

Defining $\tau_s = 1/k_B T$ as we have done all along and comparing (22) with (21) clearly proves the point made earlier in this section. That is in the temperature limit, $D \gg k_B T$,

and in the presence of a barrier in the potential, it is the Monte Carlo method which is faster than the Langevin method. In fact, the presence of the exponential factor in (21) ensures that the Monte Carlo method is very much better than the Langevin method for this case.

5. The effect of the step time on the Langevin method

As mentioned in the introduction, the Langevin equation (3) has to be replaced by a recurrence relation before it can be solved on a computer. The recurrence relation has a form

$$\theta_{n+1} = \theta_n - (\partial H / \partial \theta)_{\theta = \theta_n} - f_n \Delta t \tag{23}$$

where θ_{n+1} is the new value of θ . θ_n is the value of θ at the n th step and the time is discretised in steps of Δt , i.e. $t = n \Delta t$. Following Bray and Moore (1982) we have assumed that the random noise $f_n \Delta t$ has a Gaussian distribution with zero mean and variance $2\Delta t k_B T$. Also it is assumed that values of f_n for two different values of n are independent. Using the above distribution for $f_n \Delta t$ it is obvious that f_n itself has to have a Gaussian distribution of the form

$$P(f_n) df_n = (\Delta t / 4\pi k_B T)^{1/2} \exp(-\Delta t f_n^2 / 4k_B T) df_n \tag{24}$$

The probability distribution of θ_{n+1} depends on both the distribution of θ_n and that of f_n . It is given by

$$P_1(\theta_{n+1}) = \iint P_2(\theta_n) P(f_n) \delta(\theta_{n+1} - \theta_n + (\partial H / \partial \theta - f_n) \Delta t) df_n d\theta_n \tag{25}$$

Using the integral representation of a δ function, equation (25) becomes

$$P_1(\theta_{n+1}) = \iiint P_2(\theta_n) \exp[iu(\theta_{n+1} - \theta_n + (\partial H / \partial \theta) \Delta t - f_n \Delta t)] (\Delta t)^{1/2} \times \exp(-\Delta t f_n^2 / 4k_B T) df_n d\theta_n du / 2\pi (4\pi k_B T)^{1/2} \tag{26}$$

Now, the integral in f_n followed by the integral in u can be evaluated to give

$$P_1(\theta_{n+1}) = \int \frac{\exp[-(\theta_{n+1} - \theta_n + (\partial H / \partial \theta) \Delta t)^2 / 4k_B T \Delta t]}{(4\pi k_B T \Delta t)^{1/2}} P_2(\theta_n) d\theta_n \tag{27}$$

In order to simplify the calculation, from now on we shall take $H(\theta) = \frac{1}{2}h\theta^2$. This is a reasonable assumption to make if one is dealing with any single-well potential in the low-temperature limit. One can now proceed to derive the Fokker-Planck equation from (27). In the limit $\Delta t \rightarrow 0$ the equation would be the same as (10) with a Boltzmann distribution as its steady state solution. However, if Δt is finite then some extra terms of order $\Delta t, (\Delta t)^2$, etc would appear in the equation, slightly perturbing the steady state solution away from the Boltzmann distribution. In order to calculate this new steady state solution, we have found it easier to actually solve (27) directly rather than deriving the Fokker-Planck equation with the extra terms and then trying to solve this.

Substituting a trial solution of the form

$$P_2(\theta_n) = \left(\frac{\lambda}{4\pi k_B T \Delta t} \right)^{1/2} \exp\left(\frac{-\lambda \theta_n^2}{4k_B T \Delta t} \right) \quad (28)$$

into (27) and carrying out the integration in x_n gives

$$P_1(\theta_{n+1}) = \left(\frac{1}{4\pi k_B T \Delta t} \right)^{1/2} \left(\frac{\lambda}{\lambda + \alpha^2} \right)^{1/2} \exp\left(\frac{-\lambda \theta_{n+1}^2}{4k_B T \Delta t (\alpha^2 + \lambda)} \right) \quad (29)$$

where α is given by

$$\alpha = 1 - h \Delta t.$$

If $P_1(\theta_n)$ as defined by (28) is to be a steady state solution of the equation (27) then one requires distribution (29) to have the same form as (28), i.e.

$$-\lambda(\alpha^2 + \lambda)^{-1} = -\lambda.$$

Thus

$$\begin{aligned} \lambda &= 1 - \alpha^2 \\ &= 2h \Delta t - h^2(\Delta t)^2. \end{aligned} \quad (30)$$

Substituting (30) into (28) one has the steady state solution of equation (27):

$$P(\theta) = \left(\frac{2h \Delta t - h^2(\Delta t)^2}{4\pi k_B T \Delta t} \right)^{1/2} \exp\left(\frac{h^2 \Delta t \theta^2}{4k_B T} \right) \exp\left(\frac{-h\theta^2}{2k_B T} \right). \quad (31)$$

It can be seen that this solution is not the Boltzmann distribution if Δt is finite. However, if the limit $\Delta t \rightarrow 0$ is taken then one obtains

$$P(\theta) = \left(\frac{h}{2\pi k_B T} \right)^{1/2} \exp\left(\frac{-h\theta^2}{2k_B T} \right) \quad (32)$$

which is just the expected Boltzmann distribution. Only retaining the terms up to and including Δt , equation (31) can be written as

$$P(\theta) = \left(1 - \frac{1}{4} h \Delta t + \frac{1}{4} \frac{h^2 \theta^2}{k_B T} \Delta t \right) \left(\frac{h}{2\pi k_B T} \right)^{1/2} \exp\left(\frac{-h\theta^2}{2k_B T} \right). \quad (33)$$

The first term in the above expression gives distribution (32) and the next two terms are the leading extra terms that appear due to Δt being finite. With the help of (31) and (32) one can also calculate the error produced in a given quantity of interest. For example consider $\langle \theta^2 \rangle$. According to (31) the value of this quantity would be $(k_B T/h)(1 - h \Delta t/2)^{-1}$ whereas the true value given by distribution (32) is $k_B T/h$. Hence, a relative error of $\frac{1}{2} h \Delta t$, (up to first order in Δt), has been introduced into the quantity $\langle \theta^2 \rangle$. Note that this type of error is present in addition to the random error which arises as a result of the averaging process over the steps and also the error due to the influence of the initial starting state (errors also present in the Monte Carlo method). The random statistical error and the influence of the initial condition can both be reduced if one averages over larger and larger numbers of steps. But the error introduced by discretising the time in the Langevin equation is not reduced by increasing the number of steps. This must be considered as a disadvantage of the Langevin method compared to the Monte Carlo method. The way to reduce this error is to

introduce extra terms into the Langevin equation as has been suggested by Parisi (1980), or to use a more refined expression for the derivative (Drummond *et al* 1982). One might think that a similar kind of error must also exist in the Monte Carlo method. After all the time in the master equation (7) is continuous whereas the Monte Carlo steps in a computer are discrete. However, this is not so and as long as the transition probabilities are defined such that they satisfy the detailed balance equation, the system will approach the correct equilibrium distribution (Muller-Krumbhaar and Binder 1973).

In the last two sections we compared various relaxation times for both the Langevin and the Monte Carlo method but little attention was paid to the effect of step time. With the aid of the calculations made in this section we are in a better position to compare the two methods, at least for the case of a single well, by taking the step time into account. To do so, first we need to have criteria for choosing Δt in the Langevin method. We assume that the relative error introduced in $\langle \theta^2 \rangle$ due to discretised time must be equal to less than ξ . That requirement leads to the following restriction on the value of Δt

$$\Delta t \leq 2\xi/h. \quad (34)$$

In § 3 the dominant relaxation time for the Langevin case and a single-well potential was shown to be $1/h$. Assuming that this is so even for finite but small values of Δt , then the number of steps required for the system to get to equilibrium would be given by

$$\begin{aligned} M &= \frac{\tau_r}{\Delta t} \\ &= \frac{1/h}{2\xi/h} = \frac{1}{2\xi}. \end{aligned} \quad (35)$$

Thus, in order to reduce the error due to discretising the time one has to have a smaller step time which simply means that the system will require a greater number of steps to get to the equilibrium. For the Monte Carlo case without restriction M is given by

$$\begin{aligned} M &= \tau_r/\tau_s \\ &= \frac{1}{3}(\pi^3 h/2k_B T)^{1/2} \end{aligned} \quad (36)$$

where τ_r is the relaxation time and was shown to have a lower bound of $\frac{1}{3}\tau_s(\pi^3 h/2k_B T)^{1/2}$ in § 3. Comparing (35) and (36), one can see that the number of steps required for achieving equilibrium in the Monte Carlo case with no restriction is going to be larger than that for the Langevin method, at very low temperatures, due to the $T^{-1/2}$ dependence in (36). However, the temperature at which this happens decreases with decreasing ξ .

For the Monte Carlo method with restriction τ_r is proportional to $\tau_s = (k_B T)^{-1}$. One can immediately see that M becomes independent of temperature in this case, similar to that for the Langevin method.

A similar calculation for double-well potential could also be done if one could derive an equation like (27) and obtain the solution to it. We have found this to be a rather difficult task. Whatever the result might be though, we feel that the exponential factor $\exp(D/k_B T)$ appearing in the relaxation for the spin in a double-well potential in the Langevin case, is going to ensure that the Monte Carlo method will be the more efficient of the two in the low-temperature limit.

6. Summary and conclusion

In order to reduce the error caused by the influence of the initial configuration when the equilibrium properties of a system are being studied using computer simulation, one has to omit the first few steps from the averaging process. The number of steps to be omitted depends directly on the longest relaxation time of the system.

Langevin and Monte Carlo dynamics of a single planar spin were compared by solving the Langevin and the master equation in the low-temperature limit in order to see which had the smaller longest relaxation time. The time scale for the Monte Carlo method is defined by having τ_s (step size) equal to $k_B T$. It is shown that this choice makes the two methods consistent in the high-temperature limit.

It was found that the spin interacting with a single-well potential has a relaxation time independent of the temperature, in the low-temperature limit, when the Langevin dynamic is considered. For the Monte Carlo method without any restriction on the maximum allowed change in the angles, a variational calculation gave a lower bound which was proportional to $T^{-3/2}$ for the relaxation time in the same temperature limit. These results show that the Langevin method is faster when one is dealing with single-well potentials in low-temperature limits. The Monte Carlo method could be improved by ensuring that the change in the angle at each step is not greater than a certain upper limit. It was argued that for the best result this upper limit had to be of order $(\beta h)^{-1/2}$. In this case a variational calculation gave a lower bound proportional to T^{-1} for the relaxation time in the low-temperature limit.

One can make a better comparison between the two methods if one also takes into account the effect of the step size, i.e. calculate the number of steps required for the system to reach equilibrium for each of the two methods above. For both the Monte Carlo case with restriction and the Langevin method, this is independent of temperature. However, it was shown that for a finite step size (Δt), the equilibrium distribution deviated from the Boltzmann distribution in the case of the Langevin method. This introduced a relative error of the order $\frac{1}{2}h \Delta t$ in the quantity $\langle \theta^2 \rangle$. Thus in order to reduce this error one has to make Δt as small as possible. This means a larger number of steps (which is equal to relaxation time divided by the step size), is required for the equilibrium to be achieved. Thus it appears that unless there is a need to compute correlation functions (Parisi 1980) or explicit time dependence (Bray and Moore 1982) the Monte Carlo method is the method of choice.

When a double-well potential was considered it was found that the relaxation time for the Langevin case varied as $\exp(D/k_B T)$ as $T \rightarrow 0$, D being the height of the barrier in the potential. For the Monte Carlo method (with no restriction) the relaxation time had the same temperature dependence as the single potential case, that is $T^{-3/2}$. Thus introduction of a barrier into the potential causes the Langevin dynamic to become much slower but leaves the relaxation time for the Monte Carlo method almost unchanged. These results clearly show that for any potential with one or more barriers in it the Monte Carlo method is the more efficient of the two.

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Appendix I

In this appendix we present the details of the variational calculations which lead to equation (17). Multiplying both sides of equation (15) by a function $\exp(-\frac{1}{2}\beta h \cos \theta)$ and defining

$$g_\lambda(\theta) = f_\lambda(\theta) \exp(-\frac{1}{2}\beta h \cos \theta)$$

gives

$$-\lambda g_\lambda(\theta) = \int_{-\pi}^{+\pi} K(\theta, \theta') \exp(-\frac{1}{2}\beta h \cos \theta) \exp(+\frac{1}{2}\beta h \cos \theta') g_\lambda(\theta') \tag{A1.1}$$

where $K(\theta, \theta')$ is given by (16). Equation (A1.1) is a new integral equation with a kernel $K(\theta, \theta') \exp(-\frac{1}{2}\beta h \cos \theta) \exp(+\frac{1}{2}\beta h \cos \theta')$ which is now symmetric in θ and θ' . Thus, according to the Hilbert-Schmidt theory its eigenfunctions are orthogonal. The first eigenstate is known. This is

$$g_0(\theta) = f_0(\theta) \exp(-\frac{1}{2}\beta h \cos \theta) = \exp(\frac{1}{2}\beta h \cos \theta).$$

According to the variational procedure if $g_1(\theta)$ is any arbitrary function orthogonal to $g_0(\theta)$, then

$$\lambda \leq \left(- \int_{-\pi}^{+\pi} \int_{-\pi}^{+\pi} g_1(\theta) K(\theta, \theta') \exp(-\frac{1}{2}\beta h \cos \theta) \exp(+\frac{1}{2}\beta h \cos \theta') g_1(\theta') d\theta' d\theta \right) \times \left(\int_{-\pi}^{+\pi} \{g_1(\theta)\}^{-2} d\theta \right)^{-1} \tag{A1.2}$$

where λ is the first non-zero eigenvalue. Trying

$$g_1(\theta) = \exp(\frac{1}{2}\beta h \cos \theta) \sin \theta$$

which is orthogonal to the ground state $g_0(\theta)$ and with $K(\theta, \theta')$ given by (16), one can evaluate the integral in θ' to give

$$\lambda \leq \frac{(2\pi\tau_s)^{-1} \int_{-\pi}^{+\pi} \sin^2 \theta \exp(\beta h \cos \theta) (2|\theta| + 2 \int_{|\theta|}^{\pi} d\theta'' \exp[\beta h (\cos \theta'' - \cos \theta)]) d\theta}{\int_{-\pi}^{+\pi} d\theta \exp(\beta h \cos \theta) \sin^2 \theta}$$

In the low-temperature limit, $h \gg k_B T$, we have

$$\begin{aligned} \int_{-\pi}^{+\pi} \sin^2 \theta \exp(\beta h \cos \theta) d\theta &\approx 2 \int_0^{\pi} \theta^2 \exp(\beta h) \exp(-\frac{1}{2}\beta h \theta^2) d\theta \\ &= (2\pi)^{1/2} \exp(\beta h) (\beta h)^{-3/2} \end{aligned}$$

and

$$\begin{aligned} \int_{-\pi}^{+\pi} |\theta| \sin^2 \theta \exp(\beta h \cos \theta) d\theta &\approx 2 \int_0^{\pi} \theta^3 \exp(\beta h) \exp(-\frac{1}{2}\beta h \theta^2) \\ &= 4 \exp(\beta h) (\beta h)^{-2}. \end{aligned}$$

To evaluate

$$\int_{-\pi}^{+\pi} \left(\exp(\beta h \cos \theta) \sin^2 \theta \int_{|\theta|}^{\pi} \exp[\beta h (\cos \theta'' - \cos \theta)] d\theta'' \right) d\theta$$

the substitution $\theta'' = |\theta| + \alpha$ is made which leads to

$$\begin{aligned} & 2 \int_0^\pi \left(\exp(\beta h \cos \theta) \sin^2 \theta \int_0^{\pi-\theta} \exp[\beta h (\cos|\theta| \cos \alpha - \cos \theta - \sin|\theta| \sin \alpha)] d\alpha \right) d\theta \\ & \approx 2 \int_0^\pi d\theta \exp(\beta h \cos \theta) \sin^2 \theta \int_0^\infty d\alpha \exp[\beta h (-\frac{1}{2}\alpha^2 \cos|\theta| - \alpha \sin|\theta|)] \\ & = 2 \int_0^\infty d\theta \exp(\beta h) \exp(-\frac{1}{2}\beta h \theta^2) \theta^2 (\beta h \theta)^{-1} = 2 \exp(\beta h) (\beta h)^{-2}. \end{aligned}$$

We have treated the limit $\pi - \theta$ as ∞ when evaluating the integral in α which is not a good approximation if $\theta \approx \pi$. However, the term $\exp(\beta h \cos \theta) \sin^2 \theta$ which appears in the integral ensures that the contribution from the region $\theta \approx \pi$ towards the final answer is negligible in the low-temperature limit. Hence, we have

$$\lambda \leq 3\tau_s^{-1} (2k_B T / \pi^3 \hbar)^{1/2}.$$

Appendix 2

In this appendix we calculate the relaxation time required for the equilibrium to be achieved between two wells, assuming that equilibrium has already been established within each well. The transition probabilities are those governed by the Metropolis algorithm (7). The double-well potential (2) has one minima at $\theta = 0$ and one at $\theta = \pi$ (or $-\pi$) and maxima at $\theta = -\frac{1}{2}\pi$ and $\theta = \frac{1}{2}\pi$. The probability of being in the well about $\theta = 0$ is given by

$$\begin{aligned} n_1 &= \int_{-\pi/2}^{+\pi/2} P(\theta) d\theta = \int_{-\pi/2}^{+\pi/2} P(0) \exp[-\beta(V(\theta) - V(0))] d\theta \\ &\approx I_1 P(0) \exp(\beta V(0)) \end{aligned} \quad (\text{A2.1})$$

where $P(0)$ is the value of the probability distribution at $\theta = 0$ and we have assumed that $P(\theta)$ is given by the Boltzmann distribution within the well. I_1 is given by

$$I_1 = (2\pi / \beta V''(0))^{1/2} \exp(-\beta V(0)). \quad (\text{A2.2})$$

In a similar way, the probability of being in the well about $\theta = \pi$ (or $-\pi$) is given by

$$\begin{aligned} n_2 &= \int_{-\pi}^{-\pi/2} P(-\pi) \exp[-\beta(V(\theta) - V(-\pi))] d\theta \\ &\quad + \int_{+\pi/2}^{\pi} P(\pi) \exp[-\beta(V(\theta) - V(\pi))] d\theta \\ &\approx I_2 P(\pi) \exp(\beta V(\pi)). \end{aligned} \quad (\text{A2.3})$$

Note that due to periodic boundary conditions $P(\pi) = P(-\pi)$. I_2 is defined as

$$I_2 = (2\pi / \beta V''(\pi))^{1/2} \exp(-\beta V(\pi)). \quad (\text{A2.4})$$

Now we need to calculate the total transition rate from the first well into the second one and *vice versa*. We shall refer to these as ω_{12} and ω_{21} respectively. In order to obtain ω_{12} we have to get the sum of the transitions made from all the states in the first well into a particular state in the second well and then we have to sum this over

all the states in the second well. This is just the integral

$$\omega_{12} = \int_{\theta_2 = \pi/2}^{\theta_2 = \pi} \int_{\theta_1 = -\pi/2}^{\theta_1 = \pi/2} P(\theta_1) \omega(\theta_1, \theta_2) d\theta_1 d\theta_2 + \int_{\theta_2 = -\pi}^{\theta_2 = -\pi/2} \int_{\theta_1 = -\pi/2}^{\theta_1 = \pi/2} P(\theta_1) \omega(\theta_1, \theta_2) d\theta_1 d\theta_2.$$

With $P(\theta_1) = P(0) \exp[-\beta(V(\theta_1) - V(0))]$ and $\omega(\theta_1, \theta_2)$ given by (7), each of the above integrals breaks into more integrals. These can quite easily be evaluated to give

$$\omega_{12} = [8P(0)/\beta V''(0)]\tau_s^{-1} \tag{A2.5}$$

and in a similar way

$$\omega_{21} = [8P(\pi)/\beta V''(\pi)]\tau_s^{-1}. \tag{A2.6}$$

Now n_1 , the probability of being in the first well satisfies the simple equation

$$\dot{n}_1 = \omega_{21} - \omega_{12}. \tag{A2.7}$$

Also we have $n_2 = 1 - n_1$. Thus by expressing ω_{21} and ω_{12} both in terms of n_1 , we will have a differential equation for n_1 which can be solved to give us the relaxation time required. To do so substitute (A2.5) and (A2.6) into (A2.7):

$$\dot{n}_1 = 4(\beta h)^{-1} \tau_s^{-1} (P(\pi) - P(0))$$

where we have also used the fact that $V''(0) = V''(\pi) = 2D$ for the potential $D \sin^2 \theta$. Now using (A2.1) and (A2.3) we have

$$P(\pi) = n_2 \exp(-\beta V(\pi)) I_2^{-1} = n_2 I_2^{-1}$$

$$P(0) = n_1 \exp(-\beta V(0)) I_1^{-1} = n_1 I_1^{-1}$$

which when substituted into (A2.8) gives

$$\dot{n}_1 = 8(\beta V''(0))^{-1} \tau_s^{-1} [(1 - n_1) I_2^{-1} - n_1 I_1^{-1}].$$

Solving the above differential equation gives a relaxation time

$$\tau_r = [4(\beta D)^{-1} \tau_s^{-1} (I_1^{-1} + I_2^{-1})]^{-1}.$$

With I_1 and I_2 defined by (A2.2) and (A2.4) this becomes

$$\tau_r = \frac{1}{8} (\pi \beta D)^{1/2} \tau_s.$$

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