Monte Carlo Methods Applied to Quantum-Mechanical Order-Disorder Phenomena in Crystals

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1. The Metropolis Method in Classical Statistical Mechanics

Many years ago, John Hammersley induced and encouraged me to work on this application of Monte Carlo as my doctoral research topic; as it seems that some physicists have recently become interested in the idea after its spending a long period in oblivion, it may be worth dusting off and explaining again.

The idea stems from a technique originally developed in 1953 (Metropolis et al. 1953; see also Hammersley and Handscomb 1964, Chapter 9) by Metropolis et al. (here referred to as $\mathrm{MR^2T^2}$) for the study of the equation of state of a hard-sphere gas model. Suppose that one has a physical system that can occupy any of a [large] number of possible configurations C, each having an energy given by the Hamiltonian function $H(C)$. According to the laws of classical statistical mechanics, when at temperature T the system occupies each possible configuration C with a probability proportional to

$$P(C) := \mathrm{e}^{-\beta H(C)}, \tag{1.1}$$

where $\beta := (kT)^{-1}$, k being Boltzmann's constant; the expected value of any observable $\phi(C)$ (including $H(C)$ itself) is thus given by the expression

$$\mathrm{E}\phi(C) = \frac{\sum_C \phi(C)P(C)}{\sum_C P(C)}. \tag{1.2}$$

To evaluate (1.2) directly is prohibitively expensive, and needlessly extravagant since all but a few terms in each summation are negligible unless T is very large. The form of (1.2) suggests, however, that one should be able to evaluate it approximately by a sampling ('Monte Carlo') method — if one could somehow easily generate a sample (with replacement) of configurations from a probability distribution in which configuration C occurred with probability proportional to $P(C)$, the sample average of $\phi(C)$ would then be an unbiassed estimator of (1.2). The ingenious technique put forward in MR^{2}T^2 generates such a sample by performing a 'random walk' through configuration space: starting from an arbitrary configuration C_0, one generates a sequence of configurations C_1, C_2, ..., each one move away from its predecessor, according to the following rules:

Let $A(C)$ denote the set of all configurations accessible from C in one move; assume that a 'move' is defined so that:

- if $C' \in A(C)$ then $C \in A(C')$;
- the size of $A(C)$ is independent of C;
- there is no proper subset Σ of configurations such that

$$\bigcup_{C \in \Sigma} A(C) \subseteq \bigcup_{C \in \Sigma} C.$$

Having arrived after j moves at C_j, select a new configuration C'_j at random from a uniform distribution on $A(C_j)$.

If $P(C'_j) \geq P(C_j)$, then take $C_{j+1} = C'_j$.

If $P(C'_j) < P(C_j)$, so that the chosen move would take one to a higher-energy configuration, then draw a random number ξ_j from a uniform distribution on $[0, 1]$; if $\xi_j < P(C'_j)/P(C_j)$, then again take $C_{j+1} = C'_j$; otherwise take $C_{j+1} = C_j$, so that the previous configuration is repeated.

These rules can easily be shown to give rise to an irreducible acyclic Markov chain in which the one-step transition probabilities $\Pr(C \to C')$ satisfy the equation

$$P(C)\Pr(C \to C') = P(C')\Pr(C' \to C) \quad \forall C, C' : \ C' \in A(C), \tag{1.3}$$

so that

$$P(C) = \sum_{C'} P(C')\Pr(C' \to C) \quad \forall C, \tag{1.4}$$

and the chain has an equilibrium distribution proportional to $P(C)$.

Notice that in carrying out this procedure it is never necessary to evaluate $P(C)$ or the Hamiltonian function completely, since

$$\frac{P(C')}{P(C)} = \mathrm{e}^{-\beta(H(C')-H(C))}, \tag{1.5}$$

so that all that one needs to compute is the change in energy $H(C'_j) - H(C_j)$ produced by each proposed move. In the original hard-sphere gas model of MR^{2}T^2, for instance, each move consists of shifting just one sphere to a new position — the change in energy and the probability of accepting the move depend only on this sphere and those with which it comes in contact.

This procedure is thus very easy to implement. It is very effective in generating a suitable sample of configurations. There are only two real difficulties:

- starting from a low-probability configuration, it may take many moves to reach a high-probability one, so that there is some problem in deciding how many initial steps of the chain should be discarded as transient and unrepresentative before one begins sampling;
- since the sample is by its very nature highly correlated, it is not easy to make a statistical assessment of the error in using the sample average of $\phi(C_j)$ as an estimator of $\mathrm{E}\phi(C)$.

The principle of $\mathrm{MR}^2\mathrm{T}^2$ has been applied to the study of order-disorder phenomena in binary alloys (cf. Fosdick 1959) and in the Ising model of a ferromagnet or antiferromagnet (cf. Ehrman et al. 1960).

The Ising model, for instance, models the ferromagnet by a fairly large array of n sites on a crystal lattice, the 2^n configurations C then being all possible assignments of a positive or negative spin to each site. On the assumption that each spin interacts only with its nearest neighbours and with an external (uniform) magnetic field, the Hamiltonian takes the form[1]

$$H(C) = -J(n_{++} + n_{--} - n_{+-}) - \mu\mathcal{H}(n_+ - n_-), \tag{1.6}$$

(omitting an arbitrary constant term) where n_+ and n_- are respectively the numbers of positive and negative spins in the configuration C, and n_{++}, n_{--} and n_{+-} the numbers of nearest-neighbour pairs whose spins are respectively both positive, both negative, and one of each; equivalently

$$H(C) = -J\sum_{\mathrm{nn}} S_i S_j - \mu\mathcal{H}\sum S_i, \tag{1.7}$$

where $\sum_{\mathrm{nn}}$ denotes summation over all pairs of nearest neighbours and $S_i = \pm 1$, depending on the sign of the spin at the ith site. A possible move of the $\mathrm{MR}^2\mathrm{T}^2$ procedure consists of reversing the sign of any one spin; the set $A(C)$ thus consists of those configurations C' differing from C in the sign of a single spin, and $H(C') - H(C)$ is found simply by looking at that spin and its immediate neighbours.

A possible measure of long-range order is the value of

$$\phi_L(C) := \left(\sum S_i\right)^2 \Big/ n^2. \tag{1.8}$$

In a completely-ordered configuration, such as occurs when $T = 0$, $\phi_L(C) = 1$, while in a random configuration ($T = \infty$), $\mathrm{E}\phi_L(C) = 1/n$. As the dimensions of the lattice tend to infinity, the latter expectation tends to zero, and there is a critical temperature T_c such that $\mathrm{E}\phi_L(C) \to 0$ whenever

[1] The coefficient J represents the internal interaction, $J > 0$ for a ferromagnet or $J < 0$ for an antiferromagnet; μ is the Bohr magneton; $\mathcal{H}$ represents the external field.

$T > T_c$. On finite lattices the transition is more blurred, nevertheless, a transition between ordered and disordered behaviour is discernable even on fairly small lattices (see Figs. 1, 2), and can be picked up by the Monte Carlo method (Ehrman et al. 1960).

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+-++-+++-++--+--++
--+++++-+-+--+----
--+++++------++-++
--+-+++--+-+--+---
--+-++++++-----++-
++-++---+++-+-++--
+--++----+-++++--+
---+-+-+---++++-++
--+--++----+---++-
+-++-+-+-++-----+-
+-++--+++---------
++-+++-+++---++---
-+-------------+--
+-----++-+-+++-+++
--++++-+-+++--++-+
+++++-+--+++-+++-+
+++--+---+-+------
+-+----+-+--++----
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FIG. 1. A high-temperature Ising configuration.

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-++++---+++++++---
-++++---+++++-+---
-++++++++++-------
----++++++--------
---+++++++--------
+--++++-++---+++++
+--+++++----++++++
++++++++----++++++
++++++++----++++++
----+++-----------
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------------------
--++------+-------
--++----+++-------
--++----++++------
-++++---+++++-----
-++++---++++++----
-+++----+++++++---
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FIG. 2. A low-temperature Ising configuration.

2. Extension to a Quantum-Mechanical System

The Ising model is based on nearly-classical mechanics and does not properly represent the quantum mechanics of magnetic interactions; better models to adopt are the XY model and the Heisenberg model, in which quantum theory is applied without compromise.

In quantum statistics, the Hamiltonian H represents not a function, but a linear operator on distributions over configuration space (for classical systems H would be a diagonal operator); suppose it to take the form

$$H = H_0 + \sum_{i=1}^{N} H_i, \tag{2.1}$$

where H_0 commutes with each H_i but otherwise H_i may or may not commute with H_j. The expectation of any linear operator Φ is then given by the expression

$$\begin{aligned}\langle \Phi \rangle &= \frac{\operatorname{trace}\{\Phi \exp(-\beta H)\}}{\operatorname{trace}\{\exp(-\beta H)\}} \\ &= \frac{\sum_{r=0}^{\infty} (-\beta)^r / r! \sum_{Z_r} \operatorname{trace}\{\Phi H_{i_1} \ldots H_{i_r} \exp(-\beta H_0)\}}{\sum_{r=0}^{\infty} (-\beta)^r / r! \sum_{Z_r} \operatorname{trace}\{H_{i_1} \ldots H_{i_r} \exp(-\beta H_0)\}},\end{aligned} \tag{2.2}$$

where Z_r denotes any sequence $\{i_1, \ldots, i_r\}$ of r indices in the range $1 \le i \le N$. [Z_0 is the empty sequence $\{\ \}$.]

The scheme I proposed in the early 1960s (Handscomb 1962, 1964) exploits the resemblance of (2.2) to (1.2). The key idea is no longer to require a 'configuration' to correspond directly to a physical state of the system, provided only that it is possible to assign to each such 'configuration' a weight $P(C)$ and a parameter $\phi(C)$ such that (1.2) has a meaningful value.

Take as 'configurations' C all the (infinitely many) possible sequences Z_r, $0 \le r < \infty$. If then we define

$$\phi(Z_r) := \frac{\operatorname{trace}\{\Phi H_{i_1} \ldots H_{i_r} \exp(-\beta H_0)\}}{\operatorname{trace}\{H_{i_1} \ldots H_{i_r} \exp(-\beta H_0)\}}, \tag{2.3}$$

and

$$P(Z_r) := \frac{(-\beta)^r}{r!} \operatorname{trace}\{H_{i_1} \ldots H_{i_r} \exp(-\beta H_0)\}, \tag{2.4}$$

we have

$$\langle \Phi \rangle = \mathrm{E}\phi(Z_r) = \frac{\sum_{r=0}^{\infty} \sum_{Z_r} \phi(Z_r) P(Z_r)}{\sum_{r=0}^{\infty} \sum_{Z_r} P(Z_r)}, \tag{2.5}$$

so that if one can use something like the $\mathrm{MR^2T^2}$ procedure to generate a sample of sequences with probabilities proportional to $P(Z_r)$ then the sample average of $\phi(Z_r)$ will be an unbiassed estimator of $\langle \Phi \rangle$.

In particular, it is easy to see that

$$\langle H \rangle = \langle H_0 \rangle - \langle r/\beta \rangle. \tag{2.6}$$

For this to work, one of course needs $P(Z_r)$ to yield a proper probability distribution, so that we must have

$$P(Z_r) \ge 0 \quad \forall Z_r, \tag{2.7}$$

$$\sum_{r=0}^{\infty} \sum_{Z_r} P(Z_r) < \infty. \tag{2.8}$$

We must also have

$$\phi(Z_r) \le \infty \quad \forall Z_r \tag{2.9}$$

(which is liable to be violated when $P(Z_r) = 0$). Conditions (2.7), (2.8) and (2.9) impose restrictions on the form of H. In order to be able to apply the $\mathrm{MR^2T^2}$ process, we must further define our possible moves so that (at the very least)

$$\exists Z' \in A(Z_r) : P(Z') > 0 \quad \forall Z_r : P(Z_r) > 0; \tag{2.10}$$

otherwise there is no escape from Z_r.

If all $P(Z_r) \neq 0$, then obvious possible moves are to add a single index to the beginning, to the end, or somewhere in the middle of the current sequence or else to delete the first, the last, or another index from the current sequence. The process is less likely to become 'bogged down' in a set of a few sequences if additions and deletions are at random points of the sequence. (See Lyklema 1982.) The rule for deciding whether to accept a move has to be a little more complicated than the original $\mathrm{MR}^2\mathrm{T}^2$ rule, since there are obviously more ways of extending a sequence than there are of shortening it, but it not difficult to formulate rules so that (1.3) is satisfied (Handscomb 1962).

In the case of the Heisenberg ferromagnet, with a single particle of spin $\frac{1}{2}$ on each site, the Ising Hamiltonian function (1.7) is replaced by the Hamiltonian operator

$$H = -\tfrac{1}{2} J \sum_{\mathrm{nn}} (\sigma_i, \sigma_j) - \mu \mathcal{H} \sum \sigma_i^z, \tag{2.11}$$

where σ_i is the Pauli spin-operator on the ith site and σ_i^z its component in the direction of the external field. Now if E_{ij} denotes the operator that interchanges the spins on the ith and jth sites, we may make the substitution

$$E_{ij} = \tfrac{1}{2}\{1 + (\sigma_i, \sigma_j)\} \tag{2.12}$$

to rewrite (2.11) as

$$H = -J \sum_{\mathrm{nn}} E_{ij} - \mu \mathcal{H} \sum \sigma_i^z. \tag{2.13}$$

Take $H_0 := -\mu\mathcal{H} \sum \sigma_i^z$ and $H_{ij} := -JE_{ij}$; then $H = H_0 + \sum_{\mathrm{nn}} H_{ij}$, where each H_{ij} commutes with H_0.

If we define Z_r to consist of a sequence $\{(i_1 j_1), \ldots, (i_r j_r)\}$ of nearest-neighbour pairs, and the corresponding interchanges together result in a permutation of the lattice that decomposes into the product of $K = K(Z_r)$ cycles, of lengths $a_1, \ldots, a_K$ ($a_k \geq 1$, $\sum a_k = n$), then a state of the lattice is invariant under this sequence of interchanges if and only if all lattice-sites in the same cycle of this permutation have the same spin, so that

$$\begin{aligned} P(Z_r) &= \frac{(-\beta)^r}{r!} \operatorname{trace}\{H_{i_1 j_1} \ldots H_{i_r j_r} \exp(-\beta H_0)\} \\ &= \frac{(\beta J)^r}{r!} \prod_{k=1}^{K(Z_r)} \{2\cosh(a_k L)\} \neq 0, \end{aligned} \tag{2.14}$$

where $L = \beta\mu\mathcal{H}$. The effect of adding or subtracting an interchange at the end of the sequence is clearly either to merge two cycles or to split one cycle into two; inserting or deleting an interchange elsewhere in the sequence can be shown to have a like effect. Consequently the acceptance probabilities can be made to depend only on the lengths of the cycles actually involved.

A measure of long-range order is given by $\langle \Phi_L \rangle$, where

$$\begin{aligned}\Phi_L &:= 2\left(\sum \sigma_i, \sum \sigma_i\right) \Big/ 3n(n+1) \\ &= 2\left(4\sum_{i>j} E_{ij} - n(n-4)\right) \Big/ 3n(n+1). \end{aligned} \tag{2.15}$$

This transforms into $\mathrm{E}\phi_L(Z_r)$, where

$$\phi_L(Z_r) = \frac{2}{3} \frac{\sum a_k^2 + 2\coth L \sum a_k \tanh a_k L + \{\sum a_k \tanh a_k L\}^2 - \sum a_k^2 \tanh^2 a_k L}{n(n+1)} \tag{2.16}$$

or, if $\mathcal{H} = 0$,

$$\phi_L(Z_r) = 2\sum a_k^2 \Big/ n(n+1). \tag{2.17}$$

When $T = \infty$, $\beta = 0$, we have $\langle \Phi \rangle = \operatorname{trace}\{\Phi\}/\operatorname{trace}\{\}$, so that $\langle \Phi_L \rangle = \frac{2}{n+1}$. When $T = 0$ and $\mathcal{H} = 0$, then the product of the interchanges tends towards a random permutation, so that $\langle \Phi_L \rangle = 1$. Again we expect to get a critical temperature as $n \to \infty$.

3. More Recent Work

A drawback of the scheme just presented is that it does not work for anti-ferromagnets, where $J < 0$ so that $P(Z_r)$ is not always positive, but has the sign of $(-)^r$. Also it is restricted to the Heisenberg model, and does not apply to the XY model, in which (σ_i, σ_j) is replaced by $\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y$.

These models may be treated by defining the new operator

$$h_{ij} = \sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+, \tag{3.1}$$

when we can show that

$$I - E_{ij} = h_{ij}^2 - h_{ij} \tag{3.2}$$

and

$$\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y = (\sigma_i, \sigma_j) - \sigma_i^z \sigma_j^z = 2h_{ij}. \tag{3.3}$$

Thus, instead of looking at traces of operators whose main components are of the form $\prod E_{ij}$ we can look at those of operators with components of the form $\prod h_{ij}$. Now the effect of h_{ij} on a spin state is to give zero if the spins on sites i and j are the same, and to interchange them if they differ. Consequently (provided that the lattice is such that every closed loop of nearest-neighbour bonds is of even length) trace $\prod h_{ij} \neq 0$ only if the product has an even number of interchanges with each suffix appearing an even number of times, and not always even then. It follows that in the case of the XY model we have $P(Z_r) \neq 0$ only when r is even, when $P(Z_r) \geq 0$ whatever the sign of J. Although $\prod h_{ij}$ is not now a simple permutation operator, it is possible to work out its trace mechanically, and thus implement a form of the MR^{2}T^2 algorithm — a move in this case adding or deleting *two* interchanges, which must not always be adjacent in the sequence Z_r if the space of possible sequences is to be properly sampled (Chakravarty and Stein 1982).

The Heisenberg antiferromagnet is nearly as easy (Lee et al. 1984). Shifting the energy baseline, we use (3.2) to write

$$H = J \sum_{\mathrm{nn}} (I - E_{ij}) + H_0 = J \sum_{\mathrm{nn}} (h_{ij}^2 - h_{ij}) + H_0, \tag{3.4}$$

where now, we remember, $J < 0$. Therefore

$$P(Z_r) = \frac{(\beta\,|J|)^r}{r!}\,\mathrm{trace}\Big\{\prod (h_{i_r j_r}^2 - h_{i_r j_r}) \exp(-\beta h_0)\Big\}. \tag{3.5}$$

Once again, under the same proviso, every non-zero $P(Z_r)$ will be positive.

If the lattice has closed loops of an odd number of bonds, there will be some negative weights in each case, although positive weights will normally predominate. In such a case one has to rewrite (1.2) in the form

$$\mathrm{E}\phi(C) = \frac{\sum_C \phi(C) P(C)}{\sum_C |P(C)|} \Big/ \frac{\sum_C P(C)}{\sum_C |P(C)|} \tag{3.6}$$

and estimate numerator and denominator separately — that is to say, one constructs a sample with probabilities proportional to $|P(C)|$ and uses the ratio of the sample averages of $\phi(C)\,\mathrm{sgn}\,P(C)$ and $\mathrm{sgn}\,P(C)$.

A completely different approach to the general problem (see Suzuki 1976, etc) is based on approximating the Trotter formula (Trotter 1959)

$$\exp \sum_j A_j = \lim_{n\to\infty} \Big(\prod_j \exp \frac{1}{n} A_j \Big)^n \tag{3.7}$$

by truncating the limiting process at some large n. The unanswered question here, of course, is how large n ought to be in relation to accuracy required and (possibly) the size of the lattice.

More satisfactory is the 'decoupled cell method' (Homma et al. 1986, 1987; Matsuda et al. 1988). This is closer to the original $\mathrm{MR^2T^2}$ method in that one generates a sample of spin configurations form a Markov chain, the basic move being the reversal of the spin at a lattice site. The difference is that in quantum mechanics the expression (1.1), to which the probability of configuration C is proportional, is now a diagonal element of the exponential of the operator $-\beta H$, and no longer easily determined by inspection of C. In the DCM, when one has selected the site on which the spin S_i is possibly to be reversed, one then 'decouples' the lattice into the set L_i^ν of spins which are at most ν nearest-neighbour steps from the selected site and the complementary set $\bar{L}_i^\nu$, and ignores all interactions between sites in L_i^ν and $\bar{L}_i^\nu$. One can then calculate the ratio of the probabilities that $S_i = \pm 1$, given the state of $L_i^\nu \setminus S_i$, and hence the acceptance probability for reversing S_i. In Matsuda et al. (1988) it is shown that the errors in the transition probabilities due to this approximation are $O(\beta^{\nu+1})$ for small β (high temperature T).

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