element U of the gauge group on each link. For the Z_2 gauge group (example 10.4), one assigns an action $S_\square$ to each elementary square or *plaquette* of the lattice with vertices 1, 2, 3, and 4

$$S_\square = 1 - U_{1,2}U_{2,3}U_{3,4}U_{4,1}. \tag{14.13}$$

Then, one replaces $E(x)/kT$ with βS in which the action S is a sum of all the plaquette actions S_p. More details are available at Michael Creutz's website (latticeguy.net/lattice.html). □

Although the generation of configurations distributed according to the Boltzmann probability distribution (1.345) is one of its most useful applications, the Monte Carlo method is much more general. It can generate configurations x distributed according to any probability distribution $P(x)$.

To generate configurations distributed according to $P(x)$, we accept any new configuration x' if $P(x') \ge P(x)$ and also accept x' with probability

$$P(x \to x') = P(x')/P(x) \tag{14.14}$$

if $P(x) > P(x')$.

This works for the same reason that the Boltzmann version works. Consider two configurations x and x'. If the system is thermalized, then the probabilities $P_t(x)$ and $P_t(x')$ have reached equilibrium, and so the rate $R(x \to x')$ from $x \to x'$ must equal that $R(x' \to x)$ from $x' \to x$. If $P(x') < P(x)$, then $R(x' \to x)$ is

$$R(x' \to x) = v\, P_t(x') \tag{14.15}$$

in which v is the rate of choosing $\delta x = x' - x$, while the rate $R(x \to x')$ is

$$R(x \to x') = v\, P_t(x)\, P(x')/P(x) \tag{14.16}$$

with the same v since the random walk is symmetric. Equating the two rates

$$R(x' \to x) = R(x \to x') \tag{14.17}$$

we find that the flow of probability stops when

$$P_t(x) = P(x)\, P_t(x')/P(x') = c\, P(x) \tag{14.18}$$

where c is independent of x'. Thus $P_t(x) \to P(x)$.

Sometimes the mean value $E[\mathcal{O}]$ of an observable $\mathcal{O}$ is a ratio

$$E[\mathcal{O}] = \int \mathcal{O}(x)\, Q(x)\, dx \Big/ \int Q(x)\, dx \tag{14.19}$$

of integrals with a weight function $Q(x) = \exp(i\theta(x))\,|Q(x)|$ that assumes negative or complex values and so is not a probability distribution. One then does a double Monte Carlo with $|Q(x)|$ as the probability distribution

$$E[\mathcal{O}] = \frac{\int \mathcal{O}(x)\, e^{i\theta(x)}\, |Q(x)|\, dx}{\int |Q(x)|\, dx} \Bigg/ \frac{\int e^{i\theta(x)}\, |Q(x)|\, dx}{\int |Q(x)|\, dx}\,. \tag{14.20}$$

Such double Monte Carlos may converge slowly, however.

So far we have assumed that the rate of choosing $x \to x'$ is the same as the rate of choosing $x' \to x$. In **Smart Monte Carlo** schemes, physicists arrange the rates $v_{x\to x'}$ and $v_{x'\to x}$ so as to steer the flow and speed-up thermalization. To compensate for this asymmetry, they change the second part of the Metropolis step from $x \to x'$ when $E' = E(x') > E = E(x)$ to accept conditionally with probability

$$P(x \to x') = P(x')\, v_{x'\to x} / \left[P(x)\, v_{x\to x'}\right]. \tag{14.21}$$

Now if $P(x') < P(x)$, then $R(x' \to x)$ is

$$R(x' \to x) = v_{x'\to x}\, P_t(x') \tag{14.22}$$

while the rate $R(x \to x')$ is

$$R(x \to x') = v_{x\to x'}\, P_t(x)\, P(x')\, v_{x'\to x} / \left[P(x)\, v_{x\to x'}\right]. \tag{14.23}$$

Equating the two rates $R(x' \to x) = R(x \to x')$, we find

$$P_t(x') = P_t(x)\, P(x')/P(x). \tag{14.24}$$

That is $P_t(x) = P(x)\, P_t(x')/P(x')$ which gives

$$P_t(x) = N\, P(x) \tag{14.25}$$

where N is a constant of normalization.

Example 14.3 (Highly multiple integration) You can use the general Metropolis method (14.14–14.18) to integrate a function $f(x)$ of many variables $x = (x_1, \ldots, x_n)$ if you can find a positive function $g(x)$ similar to $f(x)$ whose integral $I[g]$ you know. You just use the probability distribution $P(x) = g(x)/I[g]$ to find the mean value of $I[g]f(x)/g(x)$:

$$\int f(x)\, d^n x \approx I[g] \int \frac{f(x)}{g(x)}\, \frac{g(x)}{I[g]}\, d^n x = I[g] \int \frac{f(x)}{g(x)}\, P(x)\, d^n x. \tag{14.26}$$

□