then W can be expressed as

$$e^{-W} = e^{-\beta\mu^* N - \ln N! - \beta U_N}. \tag{15.70}$$

There are two possible ways of obtaining a trial configuration. The first involves the displacement of a selected particle; such a move is accepted or rejected according to the usual criteria, that is, by the change in the potential energy U_N. In the second possible way, we choose with equal probability whether to attempt to add a particle at a randomly chosen position in the central cell or to remove a particle that is already present. In either case, the trial configuration is accepted if W in (15.70) is increased. If W is decreased, the change is accepted with a probability equal to

$$\frac{1}{N+1} e^{\beta(\mu^* - (U_{N+1} - U_N))} \quad \text{(insertion)}, \tag{15.71a}$$

or

$$N e^{-\beta(\mu^* + (U_{N-1} - U_N))} \quad \text{(removal)}. \tag{15.71b}$$

In this approach μ^* is an input parameter, and μ is not determined until the end of the calculation when $\langle N \rangle_{\mu \mathrm{VT}}$ is obtained.

As we have discussed, the probability that a system at a temperature T has energy E is given by (see (15.53))

$$P(E, \beta) = \frac{g(E)\, e^{-\beta E}}{Z}. \tag{15.72}$$

If the density of states $g(E)$ was known, we could calculate the mean energy (and other thermodynamic quantities) at any temperature from the relation

$$\langle E \rangle = \frac{1}{Z} \sum_E E g(E) e^{-\beta E}. \tag{15.73}$$

Hence, the density of states is a quantity of much interest.

Suppose that we were to try to compute $g(E)$ by doing a random walk in energy space by flipping the spins at random and accepting all configurations that are obtained. Then the histogram of the energy $H(E)$, the number of visits to each possible energy E of the system, would converge to $g(E)$ if the walk visited all possible configurations. In practice, it would be impossible to realize such a long random walk given the extremely large number of configurations. For example, the Ising model on a 10×10 square lattice has $2^{100} \approx 1.3 \times 10^{30}$ spin configurations.

The main difficulty of doing a simple random walk to determine $g(E)$ is that the walk would spend most of its time visiting the same energy values over and over again and would not reach the values of E that are less probable. The idea of the *Wang–Landau* algorithm is to do a random walk in energy space by flipping single spins at random and to accept the changes with a probability that is proportional to the reciprocal of the density of states. That is, energy values that would be visited often using a simple random walk would be visited less often because they have a bigger density of states. There is only one problem—we don't know the density of states. We will see that the Wang–Landau algorithm estimates the density of states at the same time that it does a random walk in phase space. For simplicity, we discuss the algorithm in the context of the Ising model for which E is a discrete variable.

1. Start with an initial arbitrary configuration of spins and a guess for the density of states. The simplest guess is to set $g(E) = 1$ for all possible energies E.
2. Choose a spin at random and make a trial flip. Compute the energy before the flip, E_1, and after, E_2, and accept the change with probability

$$p(E_1 \to E_2) = \min\left(\frac{g(E_1)}{g(E_2)}, 1\right). \tag{15.74}$$

   Equation (15.74) implies that if $g(E_2) \le g(E_1)$, the state with energy E_2 is always accepted; otherwise, it is accepted with probability $g(E_1)/g(E_2)$. That is, the state with energy E_2 is accepted if a random number $r \le g(E_1)/g(E_2)$.
3. Suppose that after step (2) the energy of the system is E. (E is E_2 if the change is accepted or remains at E_1 if the change is not accepted.) Then

$$g(E) = f g(E) \tag{15.75}$$

$$H(E) = H(E) + 1. \tag{15.76}$$

   That is, we multiply the current value of $g(E)$ by the modification factor $f > 1$, and we update the existing entry for $H(E)$ in the energy histogram. Because $g(E)$ becomes very large, in practice we must work with the logarithm of the density of states so that $\ln(g(E))$ will fit into double precision numbers. Therefore, each update of the density of states is implemented as $\ln(g(E)) \to \ln(g(E)) + \ln(f)$, and the ratio of the density of states is computed as $\exp[\ln(g(E_1)) - \ln(g(E_2))]$.
4. A reasonable choice of the initial modification factor is $f = f_0 = e^1 \simeq 2.71828\ldots$. If f_0 is too small, the random walk will need a very long time to reach all possible energies; however, too large a choice of f_0 will lead to large statistical errors.
5. Proceed with the random walk in energy space until a "flat" histogram $H(E)$ is obtained, that is, until all the possible energy values are visited an approximately equal number of times. If the histogram was truly flat, all the possible energies would have been visited an equal number of times. Of course, it is impossible to obtain a perfectly flat histogram, and we will say that $H(E)$ is flat when $H(E)$ for all possible E is not less than p of the average histogram $\langle H(E) \rangle$; p is chosen according to the size and the complexity of the system and the desired accuracy of the density of states. For the two-dimensional Ising model on small lattices, p can be chosen to be as high as 0.95, but for large systems the criterion for flatness may never be satisfied if p is too close to unity.
6. Once the flatness criterion has been satisfied, reduce the modification factor f using a function such as $f_1 = \sqrt{f_0}$, reset the histogram to $H(E) = 0$ for all values of E, and begin the next iteration of the random walk during which the density of states is modified by f_1 at each step. The density of states is not reset during the simulation. We continue performing the random walk until the histogram $H(E)$ is again flat.
7. Reduce the modification factor $f_{i+1} = \sqrt{f_i}$, reset the histogram to $H(E) = 0$ for all values of E, and continue the random walk. Stop the simulation when f is smaller than a predefined value (such as $f_{\mathrm{final}} = \exp(10^{-8}) \approx 1.00000001$). The modification factor acts as a control parameter for the accuracy of the density of states during the simulation and also determines how many Monte Carlo sweeps are necessary for the entire simulation.