1 Energy histogram and density of states

Let us define the distribution $h(E_0, \beta)$ that gives the probability of configurations of energy E_0 at temperature β. For simplicity we assume that the state space is discrete (a spin system, for instance) so that the Hamiltonian takes discrete values. If this is not the case, we should simply integrate over the appropriate variables (for a fluid, for instance, we integrate over the coordinates and the momenta). Correspondingly, we assume that the possible energy values are discrete.

Formally, the distribution $h(E_0, \beta)$ is defined by

$$
\begin{aligned}
h(E_0, \beta) &= \langle \delta_{H(x),E_0} \rangle_\beta = \frac{1}{Z_\beta} \sum_x \delta_{H(x),E_0} e^{-\beta H(x)} \\
&= \frac{1}{Z_\beta} e^{\beta E_0} \sum_x \delta_{H(x),E_0}
\end{aligned}
$$

where δ_{E,E_0} is the Kronecker delta function. This function satisfies the obvious property:

$$
\begin{aligned}
\sum_{E_0} E_0^k h(E_0, \beta) &= \frac{1}{Z_\beta} \sum_{E_0} \sum_x E_0^k \delta_{H(x),E_0} e^{-\beta H(x)} \\
&= \frac{1}{Z_\beta} \sum_{E_0} \sum_x H(x)^k \delta_{H(x),E_0} e^{-\beta H(x)} \\
&= \frac{1}{Z_\beta} \sum_x H(x)^k \left(\sum_{E_0} \delta_{H(x),E_0} \right) e^{-\beta H(x)} = \langle H(x)^k \rangle_\beta
\end{aligned}
$$

In particular, the width $W(\beta)$ satisfies

$$
W(\beta)^2 = \langle H(x)^2 \rangle_\beta - \langle H(x) \rangle_\beta^2 = kT^2 C_v(T) = \hat{C}(T)
$$

The function $h(E; \beta)$ is sometimes called the *energy histogram* because it is derived from the histogram of the energy values obtained in the Monte Carlo simulation. Remember that

$$
C_v(T) = \frac{\partial E}{\partial T},
$$

from which it follows that

$$
\hat{C}(T) = -\frac{\partial E}{\partial \beta}.
$$

Since $\hat{C}(T) \sim N$, we obtain that the width of $h(E; \beta)$ scales as $\sqrt{N}$.

A related important concept is that of the *density of states $\rho(E)$*. For a system with discrete energy values we define $\rho(E)$ as the *number of states of energy E*. The origin of the name (i.e., why it is called *density*) is better understood in the continuous case, where

$$\rho(E)dE = \text{number of states with energy in } [E, E + dE].$$

In this case

$$\text{number of states with energy in } [E_1, E_2] = \int_{E_1}^{E_2} \rho(E)dE.$$

We relate $h(E, \beta)$ with $\rho(E)$

$$h(E_0, \beta) = \frac{1}{Z_\beta} e^{\beta E_0} \sum_{x, H(x) = E_0} 1$$

where the sum is only over the configurations for which $H(x) = E_0$. Each of these configurations (their number is $\rho(E_0)$) gives the same contribution, one, so that

$$h(E_0, \beta) = \frac{1}{Z_\beta} \rho(E_0) e^{-\beta E_0}.$$

This equations shows that we can estimate $\rho(E_0)$ up to a multiplicative energy-independent constant (the partition function Z_β) from the estimates of $h(E_0, \beta)$. However, the estimate is reliable only on the small energy interval centered around $\langle H \rangle_\beta$ (the average value of the Hamiltonian), of width $\sqrt{\hat{C}} \sim \sqrt{N}$.