Acceptance probability

Références

1 Acceptance probability

Consider a particle of mass \( m \) moving in a one-dimensional potential \( v(x) \). In a Monte Carlo simulation with a Metropolis algorithm, at each step of the simulation, a random and uniform move is proposed for the particle with an amplitude displacement comprised between \(-\delta\) and \(\delta\).

\( \triangledown \) 1 Write the master equation of the Monte Carlo algorithm for the probability \( P(x,t) \) of finding the particle at \( x \) at time \( t \) as a function of

\[
W(x \to x+h) = \min(1, \beta \exp(-v(x+h) + v(x)))
\]
and of \( W(x+h \to x) \). Verify that the system goes to equilibrium.

\( \triangledown \) 2 The acceptance rate is defined as the ratio of new configurations over the total number of configurations. Justify that this ratio is given by the expression

\[
P_{\text{acc}}(\delta) = \frac{1}{2R} \int_{-\infty}^{+\infty} dx \exp(-\beta v(x)) \int_{-\delta}^{\delta} dh W(x \to x+h)
\]

where \( R = \int_{-\infty}^{+\infty} dx \exp(-\beta v(x)) \).

\( \triangledown \) 3 Show that the above equation can be reexpressed as

\[
\frac{d(P_{\text{acc}}(\delta))}{d\delta} = \frac{1}{2R} \int_{-\infty}^{+\infty} dx \exp(-\beta v(x))(W(x \to x+\delta) + W(x \to x-\delta))
\]

Let us consider the following potential :

\[
v(x) = \begin{cases} 
0 & |x| \leq a, \\
+\infty & |x| > a.
\end{cases}
\]

One restricts to the case where \( \delta < a \).

\( \triangledown \) 4 Show that

\[
P_{\text{acc}}(\delta) = 1 - A\delta
\]

where \( A \) is a constant to be determined.

\( \triangledown \) 5 The mean square displacement of the position of the particle for each new configuration is given by :

\[
\langle (\Delta x)^2 \rangle = \frac{1}{2\delta R} \int_{-\infty}^{\infty} dx e^{-\beta v(x)} \int_{-\delta}^{\delta} dh h^2 \Pi(x \to x+h)
\]

Calculate \( \langle (\Delta x)^2 \rangle \) for the aforementioned potential. Infer the optimal value of \( \delta \).