Illustration of simulation

Evolution of the magnetization, 2D Ising model, $T/J=2.2$ (below $T_c$)
• $\langle M \rangle = 0$, but time scale for $M$-reversal increases with $L$
• Symmetry-breaking occurs in practice for large $L$
Magnetization distribution \( P(m) \)

The distribution depends on \( T \) and \( L \)
- single peak around \( m=0 \) for \( T>T_c \)
- double peak around \( +<m> \) and \(-<m> \) for \( T<T_c \)

Symmetry breaking (sampling of only \( m>0 \) or \( m<0 \) states) occurs in practice for large \( L \)
- because extremely small probability to go between them
Simulations with an external magnetic field

\[ E = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i \]

- here J>0 for ferromagnet
- we added minus sign in front
- a matter of taste…

For h>0, the average magnetization \( \langle M \rangle > 0 \)

Simple change in the acceptance probability

\[
P(S \rightarrow \tilde{S}_j) = \min \left[ \frac{W(\tilde{S}_j)}{W(S)}, 1 \right]
\]

\[
\frac{W(\tilde{S}_j)}{W(S)} = \exp \left[ -\frac{2J}{T} \sigma_j \left( \sum_{\delta(j)} \sigma_{\delta(j)} - h \right) \right]
\]
“Measuring” physical observables

Order parameter of ferromagnetic transition: Magnetization

\[ M = \sum_{i=1}^{N} \sigma_i, \quad m = \frac{M}{N} \]

Expectation vanishes for finite system; calculate \( \langle |m| \rangle, \langle m^2 \rangle \)

Susceptibility: Linear response of \( \langle m \rangle \) to external field

\[ E = E_0 - hM, \quad E_0 = J \sum_{i,j} \sigma_i \sigma_j \]

\[ \chi = \left. \frac{d\langle m \rangle}{dh} \right|_{h=0} \]

(we can also consider \( h > 0 \) here)

Deriving Monte Carlo estimator

\[ \langle m \rangle = \frac{1}{Z} \sum_S me^{-(E_0-hM)/T}, \quad Z = \sum_S e^{-(E_0-hM)/T} \]

\[ \chi = -\frac{dZ/dh}{Z^2} \sum_S me^{-(E_0-hM)/T} \quad + \quad \frac{1}{Z} \frac{1}{T} \sum_S mM e^{-(E_0-hM)/T} \]

\[ \frac{dZ}{dh} = \frac{1}{T} \sum_S Me^{-(E_0-hM)/T} \]
\[ \chi = \frac{1}{N} \frac{1}{T} \left( \langle M^2 \rangle - \langle M \rangle^2 \right) = \frac{1}{N} \frac{1}{T} \langle M^2 \rangle, \quad (h = 0) \]

Extrapolating to infinite size, this gives the correct result only in the disordered phase (gives infinite susceptibility for \( T < T_c \)). We can also define the susceptibility estimator as

\[ \chi = \frac{1}{N} \frac{1}{T} \left( \langle M^2 \rangle - \langle |M| \rangle^2 \right) \]

Gives correct infinite-size extrapolation for any \( T \)

**Specific heat**

\[ C = \frac{1}{N} \frac{dE}{dT} = \frac{1}{N} \frac{d}{dT} \sum_C E(C) e^{-E(C)/T} = \frac{1}{N} \frac{1}{T^2} \left( \langle E^2 \rangle - \langle E \rangle^2 \right) \]

**Correlation function**

\[ C(\mathbf{r}) = \langle \sigma_i \sigma_j (\mathbf{r}, i) \rangle \]

Average over all spins \( i \)

\[ C(\mathbf{r}) = \frac{1}{N} \sum_{i=1}^N \langle \sigma_i \sigma_j (\mathbf{r}, i) \rangle \]