1) Qualitative Ising Model problem.

a) When the temperature is above $T_c$, we expect to see a disordered system, meaning that the average magnetization is zero. However, note that for temperatures just slightly higher than $T_c$, we see the presence of some long-range fluctuations (i.e., chunks of blue and yellow), while for the temperature well above $T_c$ we see very few long-range fluctuations. When the system is quenched by bringing the temperature below $T_c$, we expect to see the system develop a net magnetization. If we do these many times with the simulation we expect to see roughly the same number of blue and yellow outcomes. This is the phenomena of “broken symmetry” because the energy is the same whether the system is blue or yellow.

b) Consider the energy situation at the interface. If the interface is diagonal, then the spins on the interface each have two nearest neighbors of their type. Thus the interface can grow or shrink without an energy penalty.

c) Occasionally we see the system become “trapped” with one band of yellow and one band of blue. In this situation, at the interface each spin is surrounded by three that are identical to it. Thus there is an energy barrier for the interface to grow or shrink. This is a situation in which, though the system energy would be lower without the presence of an interface, the kinetics of getting the interface to disappear are very slow.

2) Square lattice with fluctuations.
(2) A square lattice of \( N \) sites that forms a membrane surface. Just for the excitation of bonds the excitation is given by

\[
\mathcal{E} = \sum_{\vec{p}, \vec{r}} b_{\vec{p}, \vec{r}}^0
\]

Particles can also adsorb on the surface, which leads to another contribution to the energy.

\[
\mathcal{Z} = \sum_{\{\vec{r} = 0, \vec{r}\}} \left[ \prod_{\vec{r}} (1 - \eta_{\vec{r}} \eta_{\vec{r}+1}) \right] \exp \left( \sum_{\vec{r}} \beta \eta_{\vec{r}} \eta_{\vec{r}+1} - \beta E \sum_{\vec{r}} b_{\vec{r}}^0 \right)
\]

This term eliminates impossible

\[ \eta_{\vec{r}} \eta_{\vec{r}+1} = 1 \quad \text{implies} \quad b_{\vec{r}}^0 = 1 \]

This product eliminates the case of

\[ \eta_{\vec{r}} \eta_{\vec{r}+1} = 1, \quad b_{\vec{r}}^0 = 0 \quad \Rightarrow \quad \text{get out} \quad 0. \]

(3) At the limit \( \beta \to 0 \), set \( \eta_{\vec{r}} = 0 \), all the particles will desorb.

\[
\mathcal{Z} = \sum_{\{\vec{r} = 0, \vec{r}\}} \prod_{\vec{r}} (1 - \eta_{\vec{r}} \eta_{\vec{r}+1}) e^{-\beta E \sum_{\vec{r}} b_{\vec{r}}^0} = \sum_{\{\vec{r} = 0, \vec{r}\}} \prod_{\vec{r}} e^{-\beta E b_{\vec{r}}^0} = \sum_{\{\vec{r} = 0, \vec{r}\}} e^{-\beta E \sum_{\vec{r}} b_{\vec{r}}^0}
\]

\[
\mathcal{Z} = e^{-\beta E \sum_{\vec{r}} b_{\vec{r}}^0}
\]

\[
< E > = -\frac{\partial \mathcal{Z}}{\partial \beta} = \left[ \sum_{\{\vec{r} = 0, \vec{r}\}} e^{-\beta E b_{\vec{r}}^0} \right]^{-1} = \left[ e^{-\beta E} + 1 \right]^{-1}
\]

\[
\mathcal{Z} = \left[ e^{-\beta E} + 1 \right]^{-1}
\]
\[
\langle E \rangle = \frac{\partial}{\partial \beta} \left[ \frac{Z_N \exp \left( \beta E_0 \right)}{e^{\beta E}} \right] \\
= \frac{Z_N e^{\beta E}}{1 + e^{-\beta E}} = \frac{Z_N e^{\beta E}}{e^{\beta E} + 1} \\
\langle (E^2) \rangle = \frac{\partial^2}{\partial \beta^2} \left[ \frac{Z_N \exp \left( \beta E_0 \right)}{e^{\beta E}} \right] = \frac{Z_N e^{\beta E} \left( e^{\beta E} + 1 \right)^2 - 2 \beta e^{\beta E}}{(e^{\beta E} + 1)^2} \\
(1) \text{ we are given that} \\
Z = C \sum_{\{\sigma_n \}} \exp \left( \beta a \sum_{n=0}^{N} + \beta \sum_{n,m} \sigma_n \sigma_m \right) \\
\text{What does the partition function for an anti-ferromagnetic Ising model look like?} \\
\Phi = \sum_{\{\sigma_n \}} \exp \left[ \beta a \sum_{n=0}^{N} + \beta \sum_{n,m} \sigma_n \sigma_m \right] \\
\text{It looks the same as for a ferromagnetic Ising model, except the value of } J \text{ is negative.} \\
\text{From Problem 5.4 in Chandler, we have the correspondence between the Ising model and the lattice gas.} \\
\mu = 2mH - 2Jz \\
\varepsilon = 4J \\
\text{Note that for the 2D Ising model} \\
\frac{\beta C}{\varepsilon} = \frac{2.3J}{k_B} \Rightarrow \beta J = 0.44. \\
\text{Also note that this } \beta C \text{ is for } H=0, \text{ which implies,} \\
\mu = 2m - 2Jz. \\
\text{Hence,} \\
(\varepsilon C)_{\text{cont}} = 4 \times (0.44) = 1.76 \\
(\mu C)_{\text{cont}} = \frac{-2m \left( \frac{\mu}{\varepsilon} \right) - 2z \left( \frac{\varepsilon}{z} \right)}{z} = -\beta E Z \frac{Z}{2}
For our partition function to line up with that of a lattice gas, we must have that

\[ \tilde{K} \to -\beta E \]

\[ (\beta E)_{\text{mic}} = -\frac{\beta E z}{2} = \frac{\kappa e}{z} \]

\[ \tilde{K} \equiv (\beta E)^c = -1.76 \]

\[ (\beta E)_{\text{cont}} = -1.76 \frac{z}{2} \]

(c) What do the coexisting phases look like?

Imagine an order parameter \( \mathbf{S} \), where \( \mathbf{S} \) is a measure of checkerboard stress.

\[ \mathbf{S} \]

\[ T_c - T \]
3) Problem 5.12 from the Chandler text
4) Problem 5.13 from the Chandler text
5) Problem 5.24 from the Chandler text

\( E = 0 \) if \( J \neq 0 \) or \( E = 0 \) if \( J = 0 \)

Otherwise, we consider:

\[
\begin{align*}
E & = 0 \quad \text{if} \quad \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix} \\
& = E + \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix} \quad \text{if} \quad \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix}
\end{align*}
\]

So that the choice of (a) or (b) config is arbitrary for each partition.

The energy here is \( EN \) where \( N = 4 \) partitions

\[ Q = 2 + 2^N e^{-\beta EN} \]

\\
(c) \[ Q = \begin{cases} \sum g \phi \exp(-\beta E) & \text{if} \quad \sum g \phi \exp(-\beta E) > 0 \\
2 + 2^N e^{-\beta EN} & \text{otherwise}
\end{cases} \]

(d) \[ L = \beta \Delta \]

\[
\frac{L}{N} = \frac{\ln \left( \frac{A}{N} \right)}{\beta N} = \frac{\ln [2 + (2e^{-\beta E})]}{\beta N}
\]

\[
\text{if} \quad 2e^{-\beta E} > 1, \quad \text{then} \quad \frac{L}{N} = \frac{\ln [2 + (2e^{-\beta E})]}{\beta N}
\]

\[
\text{if} \quad 2e^{-\beta E} = 1, \quad \text{then} \quad \frac{L}{N} = \frac{\ln 3}{\beta N}
\]

\[
\text{and if} \quad 2e^{-\beta E} < 1, \quad \lim_{N \to \infty} \left( \frac{L}{N} \right) = \frac{\ln [2 + (2e^{-\beta E})]}{\beta N}
\]

\[
\text{if} \quad 2e^{-\beta E} = 1, \quad \frac{L}{N} \to \frac{3}{\beta N}
\]

\[
\text{if} \quad 2e^{-\beta E} < 1, \quad \lim_{N \to \infty} \left( \frac{L}{N} \right) = \frac{\ln [2 + (2e^{-\beta E})]}{\beta N}
\]

(e) \( T_c \) when \( 2e^{-\beta E} = 1 \):

\[
\frac{T_c}{k_B} = \frac{1}{k_B T_c}
\]

\[ T_c = \frac{\varepsilon}{k_B} \]
6) Acceptance criteria for an Ising simulation.

Since detailed balance is satisfied by the student's criterion, it is valid (it will sample states with the correct distribution). However, because so many more moves are rejected, the time needed to reach equilibrium and the time needed to generate uncorrelated states is much, much longer. Thus, the Metropolis criterion represents a far more efficient method.