The highest temperature, at which \( \frac{\partial^2 F}{\partial x^2} = 0 \), is \( k_B T_c = \frac{1}{4} \Delta \), where \( \Delta = 2(\varepsilon_{AA} + \varepsilon_{BB} - 2\varepsilon_{AB}) \)

and the corresponding value of \( x \) is \( x = \frac{1}{2} \).

Examples:
1. Al - Zn
2. Sc - He / sl \( ^3 \)He

The diagram shows a phase diagram with critical point for phase separation. The phase boundary is marked as the common tangent construction. The spinodal line is also indicated.

The diagram includes a phase diagram for Al - Zn with liquid, fcc(Al), hcp(Zn) phases. On the right, there is a phase diagram for \( ^3 \)He and \( 0.5 \times ^4 \)He with solid and liquid phases.
Order-disorder transition

Same model but $\epsilon_{AA} + \epsilon_{BB} - 2\epsilon_{AB} < 0$.

E.g. $\beta$-brass ($Cu_0.6Zn_0.4$)

Two interpenetrating simple cubic lattices

\[ \text{Cu} \quad \text{Cu} \]
\[ \ \text{Cu} \quad \text{Zn} \quad \text{Cu} \]
\[ \text{Zn} \quad \text{Cu} \quad \text{Cu} \]
\[ \text{Cu} \quad \text{Cu} \]

Low T: Cu's all on A sublattice
Zn's all on B sublattice

High T: Randomly distributed

Let fraction of Cu on A lattice be $x$ be $\frac{1}{2} + \frac{x}{2}$

Then " " on B lattice is $\frac{1}{2} - \frac{x}{2}$

$(-\frac{1}{2} < x < \frac{1}{2})$

Internal energy is

\[ \frac{Nz}{2} \left[ \frac{1}{4} (1-x^2)(\epsilon_{AA} + \epsilon_{BB}) + \frac{(1+x) + (1-x)}{4} \epsilon_{AB} \right] \]
Entropy is

\[ S = \frac{N}{2} k_B \ln \left( \frac{N}{4(1-x)} \right) ^{\frac{N}{2}} \]

\[ = 2k_B \ln \left[ \frac{N}{4(1-x)} \right] \]

\[ = 2k_B \left[ \frac{N}{2} \ln \frac{N}{2} - \frac{N}{4} (1-x) \ln \left( \frac{N}{4(1-x)} \right) \right. \]

\[ \left. - \frac{N}{4} (1+x) \ln \left( \frac{N}{4(1+x)} \right) \right] \]

\[ = -N k_B \left[ \frac{1-x}{2} \ln \left( \frac{1-x}{2} \right) + \frac{1+x}{2} \ln \left( \frac{1+x}{2} \right) \right] \]

\[ T > T_c \]

\[ T < T_c \]

\[ \frac{\partial^2 F}{\partial x^2} = +\frac{N}{4} \left( e_{AA} + e_{BB} - 2e_{AB} \right) \]

\[ + \frac{N k_B T}{1-x^2} = 0 \text{ at critical point} \]

Solution for \( \frac{\partial F}{\partial x} = 0 \)

\[ k_B T = \frac{1}{2} e_{AAA} (2e_{AB} - e_{AA} - e_{BB}) (1-x^2) \]
Highest $T_c$: $x = 0$

$$k_B T_c = \frac{3}{4} \left( 2E_{AA} - E_{AB} - E_{BB} \right)$$

Another example: lattice gas:

$N$ sites, $N_A$ atoms ($N_A = xN$)

$$U = -\frac{N^2}{2} \frac{N_A}{x} \varepsilon$$

$$\Delta = -N \left[ x \ln x + (1-x) \ln(1-x) \right]$$

$$F = U - T \Delta$$
This gives rise to "phase separation" into a dilute and a dense phase (a "gas" and a "liquid") with a liquid-gas critical point.

This will be a homework problem.

\[ k_B T_c = \frac{2}{4} \pi \frac{1}{\alpha^2} \epsilon \quad x_c = \frac{1}{2} \]

- How to measure the order-disorder transition:
- X-ray diffraction

Scattered intensity \( I(\mathbf{q}) \) at \( \mathbf{q} = \mathbf{k}' - \mathbf{k} \)

is proportional to \( \frac{g_0}{\mathbf{q}^2} |ne(\mathbf{q})|^2 \)

\( ne(\mathbf{q}) \) = electron density in the alloy.

For \( T < T_c \), \( ne(\mathbf{q}) \) has extra Fourier components corresponding to the superlattice.
Some experimental results in comparison to Ising model:

\[ M \sim M_0 - A \alpha(T - T_c) \]

Compare this with, say Fe, Co, Ni:

\[ M(T) \sim M(0) - K_1 T^{3/2} \]

So, what are the Ising model leave out?

Well, spin is a vector, not a two-valued object.

(i) It is a quantum, not a classical object.
(iii). It is a several-component vector.

This suggested to Heisenberg the "Heisenberg model"

\[ H = -J \sum_{i<j} \mathbf{S}_i \cdot \mathbf{S}_j \]

where \( \mathbf{S}_i = \text{spin} \)

\( J > 0 \) "Ferromagnetic Heisenberg model"

\( J < 0 \) "AFM Heisenberg model"

Origin of model: exchange interaction in quantum mechanics (as discussed in QM course?)

Various varieties of Heisenberg model:

"Classical" : \( \mathbf{S} \) is a classical vector with fixed length but two angular degrees of freedom

"QM" \( \mathbf{S} \) is a quantum-mechanical spin operator

In presence of a magnetic field, we again add the term \[-J \sum_i \mathbf{S}_i \cdot \mathbf{B} \]

where \( \mathbf{B}_i = g \mu_B \mathbf{S}_i \) where \( \mu_B = \frac{e^2 \hbar}{2mc} = \text{Bohr magneton} \)

\( \mathbf{S}_i = \text{spin angle} \) 
\( \mathbf{S}_i = \text{momentum operator} \)
Recall we calculated susceptibility of rotated spins in this model.

We can use this result to do mean field theory on Heisenberg model

— this will be assigned as a homework problem.

Excitations at low temperatures.

For Ising model, there is a gap

(you will show this in your current homework).

But for Heisenberg model, there is no gap.
— instead have spin waves

\[ \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \]

Ground state.

Finite

E.g. for 1D: \( H = S_i = S_0 \frac{\hat{z}}{2} \)

classical

Suppose \( S_i^2 = S_0 \frac{\hat{z}}{2} + S_i \) \( u \) small
Where does the term $-B \sum_i S_i$ come from in the Ising model? It comes from $H_{mag} = -\sum_{i=1}^N \mu_i \cdot \vec{B}$ and we just write $\vec{\mu}_i$, instead of being a vector which can point in any direction, is a variable which can take on only two values: +1 and -1.

Also, take $\vec{B} = B \hat{z}$, $\vec{\mu} = +1 \frac{\hat{z}}{2}$ or $-1 \frac{\hat{z}}{2}$.

So is a simplification of the real interaction between a spin and a magnetic field.

A couple of identities:

1. $M = -\frac{\partial F}{\partial B}$

Well $M = \frac{1}{V} \sum_i \langle S_i \rangle$.

$F = -k_B T \ln Q_N - \beta (H_0 - B \sum_i S_i) - \beta H$

where $Q_N = \text{Tr} e^{-\beta (H_0 - B \sum_i S_i)} = \text{Tr} e^{-\beta H}$

where $H_0 =$ Hamiltonian with zero magnetic field.

$M = \frac{1}{V} \sum_i \text{Tr} S_i e^{-\beta (H_0 - B \sum_i S_i)} = \frac{1}{V} \frac{\text{Tr} e^{-\beta H}}{\text{Tr} e^{-\beta H}}$
\[
\frac{\partial F}{\partial B} = -k_B T \frac{\partial}{\partial B} \ln \text{Tr} e^{-\beta H} \\
= \frac{\partial}{\partial B} \text{Tr} e^{-\beta H} (-k_B T \text{using} \frac{\partial}{\partial B} \ln \mathcal{O}) \\
= \frac{1}{\text{Tr} e^{-\beta H}} \left[ \text{Tr} \left( -\beta \frac{\partial H}{\partial B} e^{-\beta H} \right) \right] (-k_B T) \\
\]

But \( H = H_0 - B \sum_i S_i \)

So \( \frac{\partial H}{\partial B} = -\sum_i S_i \)

Thus \( \frac{\partial F}{\partial B} = -\frac{1}{\text{Tr} e^{-\beta H}} \left[ \text{Tr} \left( \sum_i S_i e^{-\beta H} \right) \right] \)

\[
= -N \left< S_i \right> \\
\]

So \( M = -\frac{1}{V} \left< \frac{\partial F}{\partial B} \right> \) QED