Advanced Statistical Mechanics

Summary/Overview

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based on the lecture
Advanced Statistical Mechanics
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Content

1 Quantum Statistics

1.1 Quantum Measurement

Physical quantities are represented by a Hermitian operator $\hat{O}$, whose eigenstates $|n\rangle$ form a complete and orthogonal basis and whose eigenvalues O_n are real. The eigenvalue equation $\hat{O}|n\rangle = O_n|n\rangle$ is equivalent to $\hat{O} = \sum_n|n\rangle O_n\langle n|$.

For an object in state $|\psi\rangle$, all values O_n are possibly measured for an observable $\hat{O}$ with probabilities $p_n = |c_n|^2 = |\langle n|\psi\rangle|^2$. The mean value can be calculated by:

$\langle\hat{O}\rangle = \sum_n p_n O_n = \sum_n|\langle n|\psi\rangle|^2 O_n = \sum_n\langle\psi|n\rangle O_n\langle n|\psi\rangle = \langle\psi|\hat{O}|\psi\rangle$.

The fluctuation (variance) is given by

$\langle(\Delta\hat{O})^2\rangle := \sum_n p_n(O_n - \langle\hat{O}\rangle)^2$

$= \sum_n p_n O_n^2 - 2\langle\hat{O}\rangle\sum_n p_n O_n + \langle\hat{O}\rangle^2\sum_n p_n = \langle\hat{O}^2\rangle - \langle\hat{O}\rangle^2$.

1.2 Density Operator

INTRODUCTION:

If an object is not prepared in a single state, but may have an state $|\psi_n\rangle$ with probability p_n, the expectation value on observable $\hat{O}$ is $\langle\hat{O}\rangle = \sum_n p_n\langle\psi_n|\hat{O}|\psi_n\rangle$.

However, one can imagine two different sets $\{|\psi_n\rangle, p_n\}$ and $\{|\phi_n\rangle, q_n\}$ which yield the same expectation value for any operator, e.g. $\sum_n p_n\langle\psi_n|\hat{O}|\psi_n\rangle = \sum_n q_n\langle\phi_n|\hat{O}|\phi_n\rangle$, hence they are equivalent. Things simplify by using

$\text{Tr}\left(\hat{O}\sum_n p_n|\psi_n\rangle\langle\psi_n|\right) = \sum_m\langle\psi_m|\hat{O}\sum_n p_n|\psi_n\rangle\langle\psi_n|\psi_m\rangle$

$= \sum_m p_m\langle\psi_m|\hat{O}|\psi_m\rangle$,

where $\text{Tr}(\hat{P}) := \sum_n\langle\psi_n|\hat{P}|\psi_n\rangle$ with a complete and orthonormal set $\{|\psi_n\rangle\}$ is the trace of the operator $\hat{P}$. Now, ensembles $\{|\psi_n\rangle, p_n\}$ and $\{|\phi_n\rangle, q_n\}$ are equivalent if and only if

$\hat{\rho} := \sum_n p_n|\psi_n\rangle\langle\psi_n| = \sum_n q_n|\phi_n\rangle\langle\phi_n|$.

Here, $\hat{\rho}$ is called *density operator/matrix* of an ensemble of quantum states. Its matrix representation ρ_{mk} is given by $\rho_{mk} = \langle m|\rho|k\rangle$, where $|n\rangle$ are the eigenfunctions of $\hat{\rho}$. Now, the expectation value of $\hat{O}$ is

$\langle\hat{O}\rangle = \text{Tr}(\hat{O}\hat{\rho}) = \text{Tr}(\hat{\rho}\hat{O}) = \text{Tr}\left(\sum_n p_n|\psi_n\rangle\langle\psi_n|\hat{O}\right)$

$= \sum_{m,n} p_n\langle\psi_m|\psi_n\rangle\langle\psi_n|\hat{O}|\psi_m\rangle = \sum_n p_n\langle\psi_n|\hat{O}|\psi_n\rangle$.

PROPERTIES:

(Here, the abbreviation *density operator = DO* is used)

1. DO's are Hermitian operators.
2. $\text{Tr}(\hat{\rho}) = \sum_n\langle\psi_n|\hat{\rho}|\psi_n\rangle = \sum_{m,n} p_m\langle\psi_n|\psi_m\rangle\langle\psi_m|\psi_n\rangle$
   $= \sum_n p_n\langle\psi_n|\psi_n\rangle = \sum_n p_n = 1$.
3. DO's are positive semi-definite, e.g.
   $\langle\phi|\hat{\rho}|\phi\rangle = \sum_n p_n|\langle\phi|\psi_n\rangle|^2 \geq 0$.
4. $\hat{\rho}$ (or ρ_{mk}) can be diagonlized such that $\hat{\rho} = \sum_n p_n|n\rangle\langle n|$, where $|n\rangle$ are $\hat{\rho}$'s eigenstates. Those p_n are of course the eigenvalues of ρ_{mk}.
5. If $|\psi\rangle = |n\rangle$, it is called a *pure state*. For a pure state is only one eigenvalue of $\hat{\rho}$ (or ρ_{mk}) 1, the others 0. Hence, for a pure state is $\text{Tr}(\hat{\rho}^2) = 1$, for a mixed $\text{Tr}(\hat{\rho}^2) < 1$.
6. The evolution of a DO is given by the Liouville equation $i\hbar\partial_t\hat{\rho} = [H, \hat{\rho}]$ (derivation: calculate $\partial_t\rho$ using product rule and substitute $\partial_t|\psi_n\rangle = \hat{H}|\psi_n\rangle/i\hbar$ using the Schrödinger eq.).

1.3 Density Operators of Thermal Ensembles

(From here on: $\rho \equiv \hat{\rho}$)

MICROCANONICAL ENSEMBLE:

In a microcanonical ensemble with fixed energy E and $W(E,N)$ *allowed* microscopic quantum states $|n\rangle$, the density operator is

$$\rho = \frac{1}{W(E,N)}\sum_n\delta_{E,E_n}|n\rangle\langle n|.$$

If $|n\rangle$ is an eigenstates of ρ it is

$$p_n = \langle n|\rho|n\rangle = \frac{\delta_{E,E_n}}{W(E,N)}.$$

The entropy is

$$S(E,N) = k\ln W = -k\sum_n p_n\ln p_n = -k\sum_n\langle n|\rho|n\rangle\ln\langle n|\rho|n\rangle$$

$$\overset{(*)}{=} -k\sum_n\langle n|\rho\ln\rho|n\rangle = -k\,\text{Tr}(\rho\ln\rho).$$

$(*)$ used that since $|n\rangle$ are the eigenfunctions of ρ, it is $\langle n|f(\rho)|n\rangle = f(\rho_n) = f(\langle n|\rho|n\rangle)$, where ρ_n is the n-th eigenvalue of ρ.

For a pure state (meaning $\rho = |\psi\rangle\langle\psi|$), the entropy vanishes:
$$S = -k\langle\psi|\rho|\psi\rangle\ln\langle\psi|\rho|\psi\rangle = -k\ln 1 = 0.$$

CANONICAL ENSEMBLE:

In a canonical ensemble, the probability of a state $|n\rangle$ with energy E_n is

$$p_n = e^{-\beta E_n}/Z.$$

Hence, the density operator is

$$\rho = \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n| = \frac{1}{Z}e^{-\beta H}.$$

Z guarantees $\text{Tr}(\rho) \overset{!}{=} 1$:

$$Z = \text{Tr}(e^{-\beta H}) = \sum_n e^{-\beta E_n}.$$

The entropy is, using in $\rho = e^{-\beta H}/Z$:

$$S = -k\,\text{Tr}(\rho\ln\rho) = -\frac{k}{Z}\text{Tr}\left(e^{-\beta H}(-\ln Z - \beta H)\right)$$

$$= \frac{k}{Z}\text{Tr}(\beta H e^{-\beta H}) + \frac{k\ln Z}{Z}\underbrace{\text{Tr}(e^{-\beta H})}_{=Z}$$

$$= \frac{1}{T}\text{Tr}\left(\frac{He^{-\beta H}}{Z}\right) + \frac{kT\ln Z}{T} = \frac{U}{T} - \frac{F}{T}.$$

Here, $U = \sum_n Z^{-1}E_n e^{-\beta E_n}$ and $F = -kT\ln Z$ was used. This is consistent with $F = U - TS$.

GRANDCANONICAL ENSEMBLE:

In a grand canonical ensemble, the probability of a state $|n\rangle$ with energy E_n and particle number N_n is

$$p_n = \frac{1}{Q}e^{-\beta(E_n - \mu N_n)}.$$

Hence, the density operator is

$$\rho = \frac{1}{Q}\sum_n e^{-\beta(E_n - \mu N_n)}|n\rangle\langle n| = \frac{1}{Q}\sum_n e^{-\beta(H - \mu\mathcal{N})}|n\rangle\langle n|$$

$$= \frac{1}{Q}e^{-\beta(H - \mu\mathcal{N})}.$$

Here, $\mathcal{N}$ is an operator with $\mathcal{N}|n\rangle = N_n|n\rangle$. Again, $\text{Tr}(\rho) \overset{!}{=} 1$, hence is has to be just the grand partition function:

$$Q = \text{Tr}(e^{-\beta(H - \mu\mathcal{N})}) = \sum_n e^{-\beta(E_n - \mu N_n)}.$$

The entropy is, using in $\rho = e^{-\beta(H - \mu\mathcal{N})}/Q$:

$$S = -k\,\text{Tr}(\rho\ln\rho) = -\frac{k}{Q}\text{Tr}\left(e^{-\beta(H - \mu\mathcal{N})}(-\beta(H - \mu N) - \ln Q)\right)$$

$$= \frac{k}{Q}\text{Tr}(\beta(H - \mu\mathcal{N})e^{-\beta(H - \mu\mathcal{N})}) + \frac{k\ln Q}{Q}\underbrace{\text{Tr}(e^{-\beta(H - \mu\mathcal{N})})}_{=\Omega}$$

$$= \frac{1}{T}\text{Tr}\left(\frac{(H - \mu\mathcal{N})e^{-\beta(H - \mu\mathcal{N})}}{Q}\right) + \frac{kT\ln Q}{T} = \frac{U - \mu N}{T} - \frac{\Omega}{T}.$$

Here, $\Omega = -kT\ln Q$ was used, which yields $\Omega = U - TS - \mu N$.

1.4 About the Von Neumann Entropy

As derived in 1.3, the so-called *von Neumann entropy* S_N is
$$S_N = -\text{Tr}(\rho \ln \rho).$$
Neglecting the k-factor, it is identical to the thermodynamic entropy. Since the $|n\rangle$-states in 1.3 are in general not the eigenstates of ρ the formula $S = -k \sum_n \langle n|\rho|n\rangle \ln\langle n|\rho|n\rangle$ is unhandy. It is more convenient to calculate the entropy in the following manner, where $f(x) = x \ln x$, $\bar{M}$ is the diagonalized matrix to a matrix M and λ_n are the eigenvalues of ρ:
$$S_N = -\text{Tr}(\rho \ln \rho) = -\text{Tr}(f(\rho)) = -\text{Tr}(\overline{f(\rho)}) = -\text{Tr}(f(\bar{\rho}))$$
$$= -\text{Tr}\begin{pmatrix} f(\lambda_1) & & 0 \\ & \ddots & \\ 0 & & f(\lambda_n) \end{pmatrix} = -\sum_n \lambda_n \ln \lambda_n.$$

1.5 Free Fermions in 3D Space

The Hamiltonian of free fermions in 3D space of volume L^3 is
$$H = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} f_{\vec{k}}^\dagger f_{\vec{k}} = \sum_{\vec{k}} E_k f_{\vec{k}}^\dagger f_{\vec{k}} = \sum_{\vec{k}} E_k N_{\vec{k}}.$$
Here, $f_{\vec{k}}^\dagger$ and $f_{\vec{k}}$ are the creation and annihilation operators, which together make up the operator $N_{\vec{k}} = f_{\vec{k}}^\dagger f_{\vec{k}}$, which gives the number of particles in the state $\vec{k}$: $N_{\vec{k}}|n\rangle = n|n\rangle$. Using the grand canonical ensemble, the density matrix is, using $N = \sum_{\vec{k}} N_{\vec{k}}$:
$$\rho = \frac{1}{Q} e^{-\beta(H-\mu N)} = \frac{1}{Q} e^{-\beta \sum_{\vec{k}}(E_k-\mu)N_{\vec{k}}} = \frac{1}{Q} \prod_{\vec{k}} e^{-\beta(E_k-\mu)N_{\vec{k}}}.$$
The partition function is
$$Q = \text{Tr}\left(\prod_{\vec{k}} e^{-\beta(E_k-\mu)N_{\vec{k}}}\right) = \prod_{\vec{k}} \text{Tr}_{\vec{k}}\left(e^{-\beta(E_k-\mu)N_{\vec{k}}}\right)$$
$$= \prod_{\vec{k}} \sum_{n=0}^{1} \langle n_{\vec{k}}|e^{-\beta(E_k-\mu)N_{\vec{k}}}|n_{\vec{k}}\rangle = \prod_{\vec{k}}\left(1 + e^{-\beta(E_k-\mu)}\right).$$
The expectation occupation of a certain state $\vec{k}_0$ is:
$$\langle n_{\vec{k}_0}\rangle = \langle N_{\vec{k}_0}\rangle = \text{Tr}\left(N_{\vec{k}_0}\rho\right) = \frac{\text{Tr}\left(N_{\vec{k}_0} \prod_{\vec{k}} e^{-\beta(E_k-\mu)N_{\vec{k}}}\right)}{Q}$$
$$= \frac{\text{Tr}_{\vec{k}_0}\left(e^{-\beta(E_{k_0}-\mu)N_{\vec{k}_0}}N_{\vec{k}_0}\right) \prod_{\vec{k}\neq \vec{k}_0} \text{Tr}_{\vec{k}}\left(e^{-\beta(E_k-\mu)N_{\vec{k}}}\right)}{\prod_{\vec{k}} \text{Tr}_{\vec{k}}\left(e^{-\beta(E_k-\mu)N_{\vec{k}}}\right)}$$
$$= \frac{\sum_{n_0=0}^{1} \langle n_0|e^{-\beta(E_{k_0}-\mu)N_{\vec{k}_0}}N_{\vec{k}_0}|n_0\rangle}{\text{Tr}_{\vec{k}_0}\left(e^{-\beta(E_{k_0}-\mu)N_{\vec{k}_0}}\right)} = \frac{e^{-\beta(E_{k_0}-\mu)}}{1 + e^{-\beta(E_{k_0}-\mu)}}.$$
The grand potential is (full derivation: *Statistical Mechanics (PHYS4031)*, Chapter 9.2), using $\Omega = -pV$:
$$\Omega = -kT \ln Q = -kT \sum_{\vec{k}} \ln\left(1 + e^{-\beta(E_k-\mu)}\right)$$
$$= -kT \int_0^\infty dE\, D(E) \ln\left(1 + e^{-\beta(E-\mu)}\right) = -\frac{2}{3}\langle H\rangle = -pV.$$
Here, the density of states in energy is $D(E) = 2V\beta^{3/2}/\sqrt{\pi}\lambda_{th}^3 \sqrt{E}$ and λ_{th} is the de-Broglie wavelength. The particle nuber is
$$\langle N\rangle = \int_0^\infty dE \frac{D(E)}{e^{-\beta(E-\mu)}+1} = \frac{2\beta^{3/2}}{\sqrt{\pi}\lambda_{th}^3} \int_0^\infty dE \frac{\sqrt{E}}{e^{-\beta(E-\mu)}+1}.$$
In the classical limit is $\langle N\rangle \lambda_{th}^3/V \ll 1$, therefore $\mu < 0, |\mu| \gg kT$:
$$\left(e^{-\beta(E-\mu)}+1\right)^{-1} \approx e^{-\beta(E-\mu)}$$
$$\Rightarrow \frac{\langle N\rangle}{V} \approx \frac{2\beta^{3/2}}{\sqrt{\pi}\lambda_{th}^3} \int_0^\infty dE\sqrt{E}\, e^{-\beta(E-\mu)} = \frac{2e^{\beta\mu}}{\sqrt{\pi}\lambda_{th}^3} \int_0^\infty dx\sqrt{x}e^{-x} = \frac{e^{\beta\mu}}{\lambda_{th}^3}$$
$$\Leftrightarrow \quad \mu = kT \ln\frac{\langle N\rangle \lambda_{th}^3}{V}.$$

1.6 Free Bosons in 3D Space

As for the fermions in 1.5, the Hamiltonian is
$$H = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} b_{\vec{k}}^\dagger b_{\vec{k}} = \sum_{\vec{k}} E_k N_{\vec{k}},$$
which yields the partition function:
$$Q = \prod_{\vec{k}} \sum_{n=0}^\infty \langle n_{\vec{k}}|e^{-\beta(E_k-\mu)N_{\vec{k}}}|n_{\vec{k}}\rangle = \prod_{\vec{k}} \sum_{n_{\vec{k}}=0}^{1} e^{-\beta(E_k-\mu)n_{\vec{k}}}$$
$$= \prod_{\vec{k}} \frac{1}{1 - e^{-\beta(E_k-\mu)}}.$$
The expectation occupation of a certain state $\vec{k}_0$ is with a similar calculation as for the fermions in 1.5:
$$\langle n_{\vec{k}_0}\rangle = \frac{\sum_{n_0=0}^\infty \langle n_0|e^{-\beta(E_{k_0}-\mu)N_{\vec{k}_0}}N_{\vec{k}_0}|n_0\rangle}{\text{Tr}_{\vec{k}_0}\left(e^{-\beta(E_k-\mu)N_{\vec{k}_0}}\right)} = \frac{\sum_{n_0=0}^\infty e^{-\beta(E_{k_0}-\mu)n_0}n_0}{\sum_{n_0=0}^\infty e^{-\beta(E_{k_0}-\mu)n_0}}$$
$$= \frac{\frac{e^{-\beta(E_{k_0}-\mu)}}{\left(1 - e^{-\beta(E_{k_0}-\mu)}\right)^2}}{\left(1 - e^{-\beta(E_{k_0}-\mu)}\right)^{-1}} = \frac{e^{-\beta(E_{k_0}-\mu)}}{1 - e^{-\beta(E_{k_0}-\mu)}} = \frac{1}{e^{\beta(E_{k_0}-\mu)} - 1}.$$
The sum is calculated $\sum_{n=0}^\infty n e^{\xi n} = \partial_\xi \sum_{n=0}^\infty e^{\xi n} = \partial_\xi\left(1 - e^\xi\right)^{-1}$. The other calculations work very similar to 1.5.

1.7 Quantum Entanglement

REDUCED DENSITY MATRIX:
Consider a system with density matrix ρ which is composed of two subsystems A and B with complete orthonormal basis $\{|n_A\rangle, |n_B\rangle\}$. If we measure an obersavble O_A only on the subsystem A, this yields
$$\langle O_A\rangle = \text{Tr}(\rho O_A) = \sum_{m,n} \langle m_A| \otimes \langle n_B|\rho O_A|n_B\rangle \otimes |m_A\rangle$$
$$= \sum_n \langle m_A| \sum_n \langle n_B|\rho|n_B\rangle O_A|m_A\rangle = \text{Tr}_A(\text{Tr}_B(\rho)O_A).$$
Obviously, the *reduced density matrix* ρ_A of a subsystem A is defined as
$$\rho_A := \text{Tr}_B(\rho).$$

ENTANGLED STATES:
A composed state
$$|\psi_{AB}\rangle = \sum_{n,m} c_{nm}|n\rangle \otimes |m\rangle$$
is separable (unentangled), if there exist coefficients a_n, b_m obeying $c_{nm} = a_n b_m$ yielding
$$|\psi_A\rangle = \sum_n a_n|n\rangle \qquad \text{and} \qquad |\psi_B\rangle = \sum_m b_m|m\rangle.$$
For Example (using $|\uparrow\downarrow\rangle := |\uparrow\rangle \otimes |\downarrow\rangle$ etc.), the state $|\uparrow\downarrow\rangle + 2|\downarrow\downarrow\rangle$ is separable, since $c_{\uparrow\uparrow} = 0 = a_\uparrow b_\uparrow; c_{\uparrow\downarrow} = 1 = a_\uparrow b_\downarrow; c_{\downarrow\uparrow} = 0 = a_\downarrow b_\uparrow; c_{\downarrow\downarrow} = 2 = a_\downarrow b_\downarrow$ yields $a_\uparrow = b_\downarrow = 1; a_\downarrow = 2; b_\uparrow = 0$ But for example for $|\psi_{AB}\rangle = |\uparrow\downarrow\rangle - 2|\downarrow\uparrow\rangle$ this is not possible and it is entangled.

ENTANGLEMENT ENTROPY:
The entanglement entropy (or simply "entanglement") is defined as the information entropy of the reduced density matrix:
$$\mathcal{E}(\rho) = -\text{Tr}(\rho_A \ln \rho_A), \qquad \rho_A := \text{Tr}_B(\rho).$$
For a pure state is $-\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_B \ln \rho_B)$. Proof: ρ_A can be diagonalized with respect to a basis of A as $\rho_A = \sum_i p_i |i_A\rangle\langle i_A|$.

2 Cluster Expansion

2.1 Cluster Expansion for Non-Ideal Classical Gases

The cluster expansion method is applicable for short range interaction particles. To be specific, the potential should decay faster than r^{-3} or the condition is

$$\lim_{|\vec{r}_i - \vec{r}_j| \to \infty} |\vec{r}_i - \vec{r}_j| u_{ij} = 0, \qquad u_{ij} := u(\vec{r}_i - \vec{r}_j).$$

The grand partition function for the classical gas is

$$Q = \sum_{N=0}^{\infty} \frac{e^{\beta \mu N}}{N! \, h^{3N}} \int d^3 p_1 \cdots d^3 p_N \int d^3 r_1 \cdots d^3 r_N e^{-\beta \sum_i \frac{p_i^2}{2m} - \beta \sum_{i<j} u_{ij}}$$

$$= \sum_{N=0}^{\infty} \frac{z^N}{N!} \int d^3 r_1 \cdots d^3 r_N \prod_{i<j} e^{-\beta u_{ij}}, \qquad z := \frac{e^{\beta \mu}}{\lambda_{th}^3}.$$

The integration over the momentum was conducted as usual for the ideal gas. Due to the coupling via u_{ij}, the spatial integration is non-trivial. Define

$$e^{-\beta u_{ij}} = 1 + f_{ij}$$

and the product can be expanded:

$$\prod_{i<j} e^{-\beta u_{ij}} = 1 + \sum f_{ij} + \sum f_{ij} f_{kl} + \cdots,$$

for example

$$e^{-\beta(u_{12} + u_{23} + u_{31})} = (1 + f_{12})(1 + f_{23})(1 + f_{31})$$

$$= 1 + f_{12} + f_{23} + f_{31} + f_{12}f_{23} + f_{23}f_{31} + f_{31}f_{12} + f_{12}f_{23}f_{31}.$$

Now, a cluster is defined as all the terms involving the same group of variable, for example

$$f_{123} := f_{12}f_{23} + f_{23}f_{31} + f_{31}f_{12} + f_{12}f_{23}f_{31}$$

is called a "cluster". Defining $f_i := 1$, it is for example for $N = 4$:

$$\prod_{i<j\leq 4} e^{-\beta u_{ij}} = f_1 f_2 f_3 f_4 + f_{12} f_3 f_4 + f_{123} f_4 + \cdots + f_{1234}.$$

Since the system has translational symmetry (all particles/interactions are identical), clusters of the same size are the same, for example

$$\int f_{123} = \int f_{234} = \int f_{124},$$

hence it is reasonable to define the coefficient

$$b_k := \frac{1}{V k!} \int d^3 r_1 \cdots d^3 r_k \, f_{12\ldots k}.$$

Thereby it is

$$\int d^3 r_1 \cdots d^3 r_N \prod_{i<j} e^{-\beta u_{ij}}$$

$$= \sum_{\substack{\text{all possible} \\ \text{partitions}}} (1! \, V b_1)^{k_1} (2! \, V b_2)^{k_2} \cdots (N! \, V b_N)^{k_N}$$

$$= \sum_{k_1 + 2k_2 + \cdots + Nk_N = N} \frac{V^{k_1} b_1^{k_1}}{k_1!} \frac{V^{k_2} b_2^{k_2}}{k_2!} \cdots \frac{V^{k_N} b_N^{k_N}}{k_N!}.$$

3 Van der Waals Gases

3.1 Order of Phase Transition

The energy, free energy, grand potential etc. are always continuous with varying temperature, volume, etc., but their differentials may not be. Here, the grand potential Ω is considered as an example, but it can also be applied to the energy U or the free energies F, G similarly.

For a macroscopic systems $V \to \infty, N \to \infty$ it reasonable to consider the pressure

$$p = -\Omega/V,$$

which is a function of density ρ (or specific volume $v := V/N = \rho^{-1}$) and T. A specific physical system is described by its equation of state $p = p(v, T)$. If now the n-th differential regarding v or T

$$\frac{\partial^n p(v, T)}{\partial \alpha^n}, \qquad \alpha = v, T,$$

is discontinuous, the phase transition is called of n-th order.

3.2 No Phase Transitions in Finite Systems

With the sole exception of Bode-Einstein condensation, all phase transitions are due to interaction between particles. Consider the two-particle potential

$$u(r) = \begin{cases} \infty & r < d \\ > u_0 & d \le r < D. \\ 0 & r \ge D \end{cases}$$

The grand partition function is

$$Q = \sum_{N=0}^{\infty} \xi^N Z_N = \sum_{N=0}^{N_0} \xi^N Z_N, \qquad \xi := e^{\beta \mu}, \qquad Z_N = \mathrm{Tr}\, e^{-\beta H}$$

(Z_N is just the partition function). But due to $u(r)$, no particles can be closer than d and hence the number of particles in a finite volume V can not exceed $N_0 \sim V/d^3$. The pressure is

$$p = \frac{kT}{V} \ln Q > 0, \quad \text{because} \quad Q = 1 + \sum_{N=1}^{N_0} \xi^N Z_N > 1.$$

The pressure is also analytical, hence there are no phase transitions.

Next, the variation of $p(v)$ is studied. The average number of particles is (take this from *Statistical Mechanics (PHYS4031)*, section 8.2):

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial \ln Q}{\partial \mu} = \frac{\partial \ln Q}{\partial \ln \xi}.$$

Using this, it follows for constant V, T:

$$\frac{\partial p}{\partial v} = \frac{\partial}{\partial (V/\langle N \rangle)} \frac{kT}{V} \ln Q = \frac{kT}{V^2} \frac{\partial \ln Q}{\partial \langle N \rangle^{-1}} = \frac{kT}{V^2} \frac{\partial \ln Q}{\partial \ln \xi} \frac{\partial \ln \xi}{\partial \langle N \rangle} \frac{\partial \langle N \rangle}{\partial \langle N \rangle^{-1}}$$

$$= \frac{kT}{V^2} \langle N \rangle \left(\frac{\partial \langle N \rangle}{\partial \ln \xi} \right)^{-1} \left(\frac{\partial \langle N \rangle^{-1}}{\partial \langle N \rangle} \right)^{-1} = -\frac{kT \langle N \rangle^3}{V^2} \langle (\Delta N)^2 \rangle^{-1}$$

$$= -\frac{kT \langle N \rangle^2}{V^2} \frac{\langle N \rangle}{\langle (\Delta N)^2 \rangle} \le 0 \qquad \text{(without approximation)}.$$

Usually is $\langle (\Delta N) \rangle \sim \sqrt{\langle N \rangle}$ and $\partial p/\partial v \approx -kT/v^2$. But if $\langle (\Delta N) \rangle \sim \langle N \rangle$ it is $\partial p/\partial v = -kT/vV \to 0, V \to \infty$ and a phase transition occurs (but not for finite systems!). Hence, phase transitions require large fluctuations!

3.3 Mean Field Derivation of van der Waals equation

For an ideal gas, the free energy is

$$F = -NkT - NkT \ln \frac{V}{N\lambda_{th}^3} \quad \Longrightarrow \quad p = -\frac{\partial F}{\partial V} = \frac{NkT}{V}.$$

Assuming the potential of 3.2, the effective volume is

$$V^* = V - Nb, \qquad b = \frac{1}{2} \frac{4\pi}{3} d^3,$$

because two particle share the volume of $2b$. The attractive interaction will reduce the energy. Assuming a uniform distribution, hence a constant $\rho = N/V$, the potential energy of the mean-field background is

$$\Delta u = \frac{1}{2} \int_{r \ge d} d^3 r\, u(r) \rho = -a \frac{N}{V}, \qquad a := -\frac{1}{2} \int_{r \ge d} d^3 r\, u(r) \ge 0.$$

Therefore, the total energy (of all particles) is lowered by $-aN^2/V$. For this approach, the free energy is

$$F = -NkT - NkT \ln \frac{V - Nb}{N\lambda_{th}^3} - \frac{aN^2}{V}$$

$$\Longrightarrow \quad p = \frac{NkT}{V - Nb} - \frac{aN^2}{V^2} = \frac{kT}{\frac{V}{N} - b} - \frac{aN^2}{V^2} = \frac{kT}{\frac{v}{N_A} - b} - \frac{aN_A^2}{v^2}$$

$$= \frac{N_A kT}{v - N_A b} - \frac{aN_A^2}{v^2} = \frac{RT}{v - b'} - \frac{a'}{v^2} \Leftrightarrow \left(p + \frac{a'}{v^2} \right)(v - b') = RT.$$

Here, $V/N = v/N_A$, N_A being Avogadro's number, as well as $a' = aN_A^2$ and $b' = N_A b$.

The critical point $(\partial p/\partial v = \partial^2 p/\partial v^2 = 0)$ is at

$$v_c = 3b, \qquad T_c = \frac{8a}{27Rb}, \qquad p_c = \frac{a}{27b^2}$$

(derivation see Statistical Mechanics (PHYS4031), section 7.3).

3.4 Critical Phenomena

As in Statistical Mechanics (PHYS4031), section 7.3, the van der Waals equation can be given as

$$\left(p + \frac{3}{v^2} \right)(3v - 1) = 8T,$$

where $p = p_{old}/p_c$ and p_{old} equals the p from section 3.3 (p, v, T are the relative quantities now). At the critical point, $p = v = T = 1$, hence quantities ρ, w, t are introduced to be small at the critical point:

$$\rho := p - 1, \qquad w := v - 1, \qquad t := T - 1.$$

If one plugs in $\rho = p - 1$ etc. into the van der Waals equation and does a Taylor expansion, the leading terms will be

$$\rho \approx 4t - 6tw - 3/2\, w^3.$$

For $t < 0$ the pressure is a symmetric 3-rd-power function. Solving $\rho - 4t = -6tw - 3/2\, w^3 = 0$ for $w \ne 0$ yields $w_\pm^2 = -4t$ and hence $w_\pm = \pm 2\sqrt{-t}$. Since w_- corresponds to the liquid phase and w_+ to the gas phase, the difference in density is

$$\rho_l - \rho_g = \frac{1}{v_l} - \frac{1}{v_g} = \frac{v_g - v_l}{v_l v_g}$$

$$= \frac{w_+ - w_-}{(w_- + 1)(w_+ + 1)}$$

$$= \frac{w_+ - w_-}{w_- w_+ + 1} \approx w_+ - w_- = 4\sqrt{-t} = 4\sqrt{|t|} = 4\sqrt{|T - 1|}$$

$$= 4\sqrt{\left| \frac{T_{old}}{T_c} - 1 \right|} = 4\sqrt{\left| \frac{T_{old} - T_c}{T_c} \right|} \sim |T_{old} - T_c|^\beta, \quad \beta = 1/2.$$

Recall, the $T = T_{old}/T_c$ is dimensionless and T_{old} is the actual temperature in Kelvin. β is a critical exponent, which is $1/2$ universally for all types of gases.
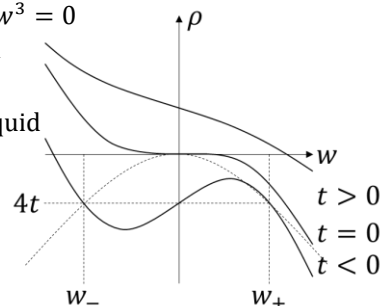
4 The Ising Model

4.1 Description of the Problem

The Hamiltonian of the Ising model is
$$H = J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - \mu B \sum_i \sigma_i^z,$$
where J is a coupling constant, B the external magnetic field and σ_i^z the z-Pauli matrix of the spin number i. The coupling is called
  antiferromagnetic for $J > 0$ and
  ferromagnetic for $J < 0$.

The eigenstates of H are $|\{s_i\}\rangle := |s_1, s_2, \ldots, s_N\rangle$, where $s_i = \pm 1$ (spin-up and -down) with eigenvalues
$$H|\{s_i\}\rangle = \left(J \sum_{\langle ij \rangle} s_i s_j - \mu B \sum_i s_i \right) |\{s_i\}\rangle.$$
In macroscopic numbers, the energy is $U(\{N_\pm\}) = J(N_{++} + N_{--} - N_{+-}) - \mu B (N_+ - N_-)$, where
$$N_{++} = \sum_{\langle ij \rangle} \delta_{s_i,1} \delta_{s_j,1}, \qquad N_- = \sum_i \delta_{s_i,-1}, \qquad \text{etc.}$$
However, the valuation of the partition function
$$Z = \text{Tr}\left(e^{-\beta H}\right) = \sum_{\{s_i\}} e^{-\beta U(\{s_i\})} = \sum_{\{N_\pm\}} W(\{N_\pm\}) e^{-\beta U(\{N_\pm\})}$$
is non-trivial at all.

4.2 Solution by Mean Field Approximation

DETERMINATION OF THE EFFECTIVE FIELD:

If there are N spins in total, N_+ pointing up and N_- down, the magnetization M and up-/down-probabilities $p_\pm$ are
$$M = \frac{N_+ - N_-}{N} = \frac{N_+ - N_-}{N_+ + N_-} = \frac{2N_+ - N}{N}, \qquad p_\pm := \frac{N_\pm}{N} = \frac{1 \pm M}{2}.$$
If one considers two neighboring spins, the probability for up-alignment is p_+^2, for down-alignment p_-^2 and for anti-alignment $2p_+ p_-$. Hence, in terms of the probabilities, the average/ expected numbers $N_\pm$ are (n = number of nearest neighbours)
$$N_{\pm\pm} = \frac{nN}{2} p_\pm^2 = \frac{nN}{8}(1 \pm M)^2, \quad N_{+-} = nN p_+ p_- = \frac{nN}{4}(1 - M^2).$$
Using this expression, the energy from 4.1 becomes
$$U(M) = \frac{JnN}{8}\left((1+M)^2 + (1-M)^2 - 2(1-M^2)\right) - \mu B N M$$
$$= \frac{JnN}{2} M^2 - \mu B N M$$
If $u := U/N$ is the average energy per spin, the effective magnetic field is given by
$$B_{\text{eff}} = -\frac{1}{\mu}\frac{\partial u}{\partial M} = B - \frac{Jn}{\mu} M.$$
So the microscopic interaction between the spins now is taken as an uniform internal macroscopic field $-nJM/\mu$, which is also called a "Bragg-Williams approximation".

MAGNETIZATION:

The energy only depends on M or N_+ instead of $\{N_\pm\}$. Therefore the partition function is much simpler:
$$Z = \sum_{N_+=0}^N W(N_+) e^{-\beta U(N_+)} = \sum_{N_+=0}^N \underbrace{\frac{N!}{N_+!(N-N_+)!} e^{-\beta U(N_+)}}_{Z_{N_+}}.$$
Of course, there is an N_+ for which Z_{N_+} is a maximum, which will dominate Z. To find this maximum, calculate $\partial \ln Z_{N_+}/\partial N_+$ and with Sterling's approximation, it is
$$\frac{\partial \ln Z_{N_+}}{\partial N_+} \approx \frac{\partial}{\partial N_+}\left(-\beta U(N_+) - N_+ \ln N_+ - (N-N_+)\ln(N-N_+)\right)$$
$$= -N\beta \frac{\partial}{\partial N_+}\left(u(N_+) + kT(p_+ \ln p_+ + p_- \ln p_-)\right)$$
$$= -N\beta \frac{\partial}{\partial N_+}(u(N_+) - Ts) = -N\beta \frac{\partial f}{\partial N_+} \stackrel{!}{=} 0,$$
where s is the entropy per spin and $f = u - Ts$ the free energy per spin. Substituting M for N_+ yields:

$$\frac{\partial f}{\partial M} = \frac{\partial}{\partial M}\left(u(M) + kT \sum_\pm p_\pm \ln p_\pm\right)$$
$$= \frac{\partial}{\partial M}\left(\frac{Jn}{2} M^2 - \mu B M + kT \sum_\pm \frac{1 \pm M}{2} \ln \frac{1 \pm M}{2}\right)$$
$$= JnM - \mu B + \frac{1}{2} kT \ln \frac{1+M}{1-M} \stackrel{!}{=} 0$$
$$\Leftrightarrow \quad M = \tanh\left(\frac{\mu B - nJM}{kT}\right).$$
For ferromagnetism ($J < 0$) and $B = 0$, this equation becomes
$$M = \tanh\left(\frac{T_c M}{T}\right), \qquad T_c := -\frac{nJ}{k} > 0.$$
As shown graphically in *Statistical Mechanics (PHYS4031)*, Section 7.4, this has three solutions for $T < T_c$. A Taylor expansion of the free energy yields ($B = 0$):
$$\frac{f(M)}{kT} = -\ln 2 + \frac{1}{2}\left(1 - \frac{T_c}{T}\right) M^2 + \frac{1}{12} M^4 + \mathcal{O}(M^6),$$
which yields that the extremum at $M = 0$ is a maximum for $T < T_c$ and a minimum for $T > T_c$.

CRITICAL EXPONENTS:

For $B = 0$ it is, using $t := (T_c - T)/T_c = 1 - T/T_c$:
$$M\frac{T_c}{T} = M\frac{1}{1-t} \approx M(1+t) \stackrel{!}{=} \text{artanh}\, M \approx M + \frac{1}{3}M^3$$
$$\Leftrightarrow \quad t \approx \frac{1}{3} M^2 \quad \Rightarrow \quad M \sim t^\beta, \quad \beta = \frac{1}{2}.$$
Deriving the equation for the magnetization w.r.t. B yields
$$\frac{d}{dB}\frac{\mu B - nJM}{kT} = \frac{\mu}{kT} + \frac{T_c}{T} M' \stackrel{!}{=} \frac{d}{dB}\text{artanh}\, M \approx M' + M^2 M'$$
$$\Leftrightarrow \quad \frac{\mu}{kT} \approx M'\left(1 - \frac{T_c}{T}\right) + M^2 M' \approx M' t + M^2 M'$$
so for $T \to T_c$ it is $M \to 0$ and hence
$$\chi := M'|_{B=0} = \frac{\mu}{kT_c t} \quad \Rightarrow \quad \chi \sim t^{-\gamma}, \quad \gamma = 1.$$
At $T = T_c$, the equation for the magnetization is
$$\frac{\mu B}{kT} + M = \text{artanh}\, M \approx M + \frac{1}{3}M^3 \quad \Rightarrow \quad B \sim M^\delta, \quad \delta = 3.$$
The specific heat capacity is
$$c_H = \frac{\partial u}{\partial T} = (JnM - \mu B)\frac{\partial M}{\partial T}$$
and since for $T > T_c$ it is $M = 0$, at $B = 0$ it is $c_H = 0$ and for $T < T_c$ it is $M \sim |t|^{1/2}$ and hence (at $B = 0$)
$$c_H \sim |t|^{1/2}\frac{1}{|t|^{1/2}} \quad \Rightarrow \quad c_H \sim |t|^\alpha, \quad \alpha = 0.$$

4.3 Exact Solution of the 1D Ising Model

Assuming periodic boundary conditions $\sigma_{N+i} = \sigma_i$ yields the Hamiltonian

$$H = J\sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - B\sum_{i=1}^{N} \sigma_i^z,$$

with eigenstates $|\{s_i\}\rangle := |s_1, s_2, \ldots, s_N\rangle$ and energies $E(\{s_i\}) = J\sum_{i=1}^{N} s_i s_{i+1} - B\sum_{i=1}^{N} s_i$, where $s_i = \pm 1$ as in 4.1. The partition function is, where s_i takes on the values ± 1:

$$Z = \sum_{\{s_i\}} e^{-\beta E(\{s_i\})} = \sum_{s_1, s_2, \ldots, s_N} \prod_{i=1}^{N} \underbrace{e^{\beta B s_i}}_{=\tilde{g}(s_i)} \underbrace{e^{-\beta J s_i s_{i+1}}}_{=f(s_i, s_{i+1})}.$$

Consider now the product

$$\tilde{g}(s_i) f(s_i, s_{i+1}) = \sum_{s_i' = \pm 1} \underbrace{\tilde{g}(s_i)\delta_{s_i s_i'}}_{=g(s_i, s_i')} f(s_i', s_{i+1}).$$

Now, g and f can be defined as matrices with components $g(s_i, s_i')$ or $f(s_i', s_{i+1})$ respectively:

$$g = \begin{pmatrix} e^{-\beta B} & 0 \\ 0 & e^{\beta B} \end{pmatrix}, \qquad f = \begin{pmatrix} e^{-\beta J} & e^{\beta J} \\ e^{\beta J} & e^{-\beta J} \end{pmatrix}.$$

This makes matrix products appear in the partition function:

$$Z = \sum_{s_1, s_2, \ldots, s_N} \sum_{s_1', s_2', \ldots, s_N'} \prod_{i=1}^{N} g(s_i, s_i') f(s_i', s_{i+1})$$

$$= \sum_{s_1, s_2, \ldots, s_N} \prod_{i=1}^{N} (gf)_{s_i, s_{i+1}} = \sum_{s_1 = \pm 1} ((gf)^N)_{s_1, s_1} = \mathrm{Tr}((gf)^N)$$

$$= \mathrm{Tr}\left((g^{1/2} g^{1/2} f)^N\right) = \mathrm{Tr}\left((g^{1/2} f g^{1/2})^N\right).$$

Note, that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$. Rewriting the matrix product like $g^{1/2} f g^{1/2} = UDU^{-1}$ defines a diagonal matrix D with the eigenvalues of $g^{1/2} f g^{1/2}$ on the diagonal positions:

$$Z = \mathrm{Tr}((UDU^{-1})^N) = \mathrm{Tr}(UD^N U^{-1}) = \mathrm{Tr}(D^N U^{-1} U) = \lambda_+^N + \lambda_-^N,$$

where $\lambda_\pm$ are the eigenvalues of D and $g^{1/2} f g^{1/2}$. The product is

$$g^{1/2} f g^{1/2} = \begin{pmatrix} e^{-\beta B - \beta J} & e^{\beta J} \\ e^{\beta J} & e^{\beta B - \beta J} \end{pmatrix}$$

and the eigenvalues can be calculated as follows:

$$\begin{vmatrix} e^{-\beta B - \beta J} - \lambda & e^{\beta J} \\ e^{\beta J} & e^{\beta B - \beta J} - \lambda \end{vmatrix}$$
$$= e^{-2\beta J} - \lambda e^{-\beta J}(e^{-\beta B} + e^{\beta B}) + \lambda^2 - e^{2\beta J} \overset{!}{=} 0,$$

$$\lambda_\pm = e^{-\beta J}\cosh\beta B \pm \sqrt{e^{-2\beta J}\frac{e^{-2\beta B} + 2 + e^{2\beta B}}{4} - e^{-2\beta J} + e^{2\beta J}}$$

$$= e^{-\beta J}\cosh\beta B \pm \sqrt{e^{-2\beta J}\frac{e^{-2\beta B} - 2 + e^{2\beta B}}{4} + e^{2\beta J}}$$

$$= e^{-\beta J}\cosh\beta B \pm \sqrt{e^{-2\beta J}\sinh^2\beta B + e^{2\beta J}}.$$

Therefore, the partition function is, since $\lambda_1 > \lambda_2$:

$$Z = \lambda_+^N + \lambda_-^N \underset{N\to\infty}{\approx} \lambda_+^N.$$

The free energy is

$$F = -kT\ln Z \approx -NkT\ln\lambda_+,$$

which is analytical for all $J, B, \beta \in \mathbb{R}$, because $\lambda_+ > 0$. Hence, there are no phase transitions. Maybe there is a phase transition for $\lambda_+ = \lambda_-$, such that the approximation is not valid. This implies

$$e^{-2\beta J}\sinh^2\beta B + e^{2\beta J} = 0,$$

which can only be fulfilled for $J < 0$, $\beta \to \infty$, $B = 0$. The phase transition would be at $T = 0$, which is not a physical phase transition. The magnetization is per spin is

$$M = -\frac{\partial F}{\partial B} \approx \frac{NkT}{\lambda_+}\frac{\partial \lambda_+}{\partial B} = \frac{N\sinh\beta B}{\sqrt{e^{4\beta J} + \sinh^2\beta B}}.$$

For no external $B = 0$, there is no spontaneous magnetization. The critical temperature is $T = 0$. The susceptibility is

$$\chi = N^{-1}\,\partial M/\partial B|_{B=0} = \beta e^{-2\beta J}.$$

4.4 Correlation Function

Although the exact solution has no phase transition, the mean field solution does. This discrepancy is due to the fluctuation. Consider the second order correlation function $f(n)$. $m = \langle \sigma_i^z \rangle$ is the magnetization per spin, which has turned out to be zero for $B = 0$ in 4.3, which will be assumed here. f does not depend on i, the following is true for any i:

$$f(n) = \langle \sigma_i^z \sigma_{i+n}^z \rangle - \langle \sigma_i^z \rangle\langle \sigma_{i+n}^z \rangle = \langle \sigma_i^z \sigma_{i+n}^z \rangle - m^2 = \langle \sigma_i^z \sigma_{i+n}^z \rangle$$

$$= \sum_{\{s_i\}} \underbrace{\frac{e^{-\beta E(\{s_i\})}}{Z}}_{\substack{\text{probability} \\ \text{of }\{s_i\}}} s_i s_{i+n} = \frac{1}{Z}\sum_{\{s_i\}} s_i \underbrace{\left(\prod_{j=1}^{n-1} \underbrace{s_{i+j}^2}_{=1}\right)}_{=1} s_{i+n} e^{-\beta E(\{s_i\})}$$

$$= \frac{1}{Z}\sum_{\{s_i\}} \left(\prod_{j=i}^{i+n-1} s_j s_{j+1}\right) e^{-\beta \sum_{k=1}^{N} J_k s_k s_{k+1}} \qquad (J_k = J\ \forall k)$$

$$= \frac{1}{(-\beta)^n Z}\sum_{\{s_i\}} \left(\prod_{j=i}^{i+n-1} \frac{\partial}{\partial J_j}\right) e^{-\beta \sum_{k=1}^{N} J_k s_k s_{k+1}}$$

$$= \frac{1}{(-\beta)^n Z}\sum_{\{s_i\}} \left(\prod_{j=i}^{i+n-1} \frac{\partial}{\partial J_j}\right) \prod_{k=1}^{N} e^{-\beta J_k s_k s_{k+1}}$$

$$= \frac{1}{(-\beta)^n Z}\left(\prod_{j=i}^{i+n-1} \frac{\partial}{\partial J_j}\right)\sum_{\{s_i\}}\prod_{k=1}^{N} f_k(s_k, s_{k+1})$$

Here, in the same way as in 4.3, a matrix

$$f_k := \begin{pmatrix} e^{-\beta J_k} & e^{\beta J_k} \\ e^{\beta J_k} & e^{-\beta J_k} \end{pmatrix}$$

was introduced and can be evaluated like an matrix product:

$$\sum_{\{s_i\}}\prod_{k=1}^{N} f_k(s_k, s_{(k+1)}) = \sum_{s_1, s_2, \ldots} f_1(s_1, s_2) f_2(s_2, s_3)\cdots = \sum_{s_1, s_3, \ldots} (f_1 f_2)_{s_1, s_3}\cdots.$$

In the same way as in 4.3, this yields:

$$f(n) = \frac{1}{(-\beta)^n Z}\left(\prod_{j=i}^{i+n-1} \frac{\partial}{\partial J_j}\right)\left(\prod_{k=1}^{N} \lambda_{+k} + \prod_{k=1}^{N} \lambda_{-k}\right)$$

$$\overset{(1)}{\approx} \frac{1}{(-\beta)^n \prod_{k=1}^{N}\lambda_{+k}}\left(\prod_{j=i}^{i+n-1} \frac{\partial}{\partial J_j}\right)\prod_{k=1}^{N} \lambda_{+k} \overset{(2)}{=} \frac{1}{(-\beta)^n}\prod_{j=i}^{i+n-1} \frac{\partial \ln\lambda_{+j}}{\partial J_j}$$

$$\overset{(3)}{=} \frac{1}{(-\beta)^n}\left(\frac{\partial \ln\lambda_+}{\partial J}\right)^n.$$

In (1) it was used that $\lambda_+ \gg \lambda_-$. In (2), all the λ_{+k} for $k \neq j$ are canceled by the λ_{+k} of the partition function. The λ_{+k} for $k = j$ survive and give $\lambda_{+j}^{-1}\,\partial\lambda_{+j}/\partial J_j = \partial\ln\lambda_{+j}/\partial J_j$. In (3) it was used that $J_j = J, \lambda_{+j} = \lambda_+\ \forall j$.

For $B = 0$ (which is assumed everywhere here), it is

$$f(n) \approx \frac{1}{(-\beta)^n}\left(\frac{\partial}{\partial J}\ln(e^{-\beta J} + e^{\beta J})\right)^n = \frac{1}{(-\beta)^n}(\beta\tanh\beta J)^n$$

$$= \tanh^n(-\beta J) \overset{!}{=} e^{-n/\xi} \qquad (\tanh(-x) = -\tanh x).$$

ξ, in the last step, is the correlation length is for $T \to 0, J < 0$:

$$\xi = \frac{-1}{\ln\tanh(-\beta J)} = \frac{-1}{\ln\dfrac{1 - e^{2\beta J}}{1 + e^{2\beta J}}} \approx \frac{-1}{\ln(1 - 2e^{2\beta J})} \approx 2e^{-2\beta J}.$$

This diverges at the critical point $T_c = 0$.

4.5 2D Ising Model: High Temperature Expansion

The Hamiltonian for the Ising model without external field

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$$

is now considered to be for a 2D lattice, where $\langle ij \rangle$ denotes nearest neighbor spins and $\sigma_i = \pm 1$. Because of the minus sign, the ferromagnetic case is now $J > 0$. The partition function is

$$Z = \mathrm{Tr}\, e^{-\beta H} = \mathrm{Tr} \prod_{\langle ij \rangle} e^{\beta J \sigma_i \sigma_j} = \mathrm{Tr} \prod_{\langle ij \rangle} \sum_{n=0}^{\infty} \frac{(\beta J \sigma_i \sigma_j)^n}{n!}$$

$$= \mathrm{Tr} \prod_{\langle ij \rangle} \left(\sum_{n=0}^{\infty} \frac{(\beta J \sigma_i \sigma_j)^{2n}}{(2n)!} + \sum_{n=0}^{\infty} \frac{(\beta J \sigma_i \sigma_j)^{2n+1}}{(2n+1)!} \right) =$$

$$= \mathrm{Tr} \prod_{\langle ij \rangle} \left(\cosh \beta J + \sigma_i \sigma_j \sinh \beta J \right)$$

$$= \cosh^{Nq/2}(\beta J)\, \mathrm{Tr} \prod_{\langle ij \rangle} \left(1 + \sigma_i \sigma_j \tanh \beta J \right)$$

$$= \left(2 \cosh^{q/2}(\kappa) \right)^N 2^{-N} \mathrm{Tr} \prod_{\langle ij \rangle} \left(1 + v \sigma_i \sigma_j \right).$$

In this derivation was used that $(\sigma_i \sigma_j)^2 = 1$ and that product constitutes of $Nq/2$ terms, were q is the number of nearest neigbours and N is the number of spins. In the last step,

$$\kappa := \beta J, \qquad v := \tanh \kappa$$

simplifies the formula. For $\kappa \ll 1 \implies v \ll 1$ (high temperature), The product term can be expanded:

$$I := 2^{-N} \mathrm{Tr} \prod_{\langle ij \rangle} (1 + v \sigma_i \sigma_j)$$

$$= 2^{-N} \mathrm{Tr} \left(1 + v \sum_{\langle ij \rangle} \sigma_i \sigma_j + v^2 \sum_{\langle ij \rangle} \sigma_i \sigma_j \sum_{\langle kl \rangle} \sigma_k \sigma_l + \cdots \right).$$

Since $\mathrm{Tr}(A + B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)$ it matters that

$$\mathrm{Tr}(\sigma_i \sigma_j) = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \sigma_i \sigma_j = 2^{N-2} \left(\sum_{\sigma_i = \pm 1} \sigma_i \right) \left(\sum_{\sigma_j = \pm 1} \sigma_j \right) = 0,$$

and for the same reason all terms like $\mathrm{Tr}(\sigma_{i_1} \sigma_{i_2} \cdots \sigma_{i_K}) = 0$ as long as all i_k are different. But consider for example:

$$\mathrm{Tr}\left((\sigma_i \sigma_j)(\sigma_j \sigma_k)(\sigma_k \sigma_i) \right) = \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_N = \pm 1} \sigma_i \sigma_j \sigma_j \sigma_k \sigma_k \sigma_i = 2^N.$$

Hence, if all spins appear twice in one term, it is not zero but $\mathrm{Tr}(\text{loop}) = 2^N$. Those terms represent spins, the bonds of which form loops. For a square lattice, this yields (note $\mathrm{Tr}(1) = 2^N$):

$$I = 2^{-N} \mathrm{Tr}(1 + \text{all closed loops})$$

$$= 1 + v^4 N_4 + v^6 N_6 + v^8 N_8 + \cdots$$

Here, N_n is the number possible loops which a made up of n bonds. For the square lattice, it is $N_4 = N$, $N_6 = 2N$ (bars made of two squares, two per spin: vertical/horizontal). For eight bonds, several shapes of loops are possible: $N_8 = N_8^{s_1} + N_8^{s_2} + \cdots$, where s_i stands for a loop-shape i. Among them is a loop made up of two separated square loops (let's call this one shape $s1$). Then, it is

$$N_8^{s_1} = N(N-5)/2 \simeq N^2 \gg N_8^{s_i}, \qquad i \neq 1$$

(for the fist square there are N possibilities, hence there are $N - 5$ left for the second square, but first and second can be exchanged, hence $1/2$).

$$Z = (2 \cosh^2 \kappa)^N \left(1 + N v^4 + 2N v^6 + \frac{N(N-5)}{2} v^8 + \cdots \right)$$

$$= \left(\frac{2}{1 - v^2} \right)^N \left(1 + N v^4 + 2N v^6 + \frac{N(N-5)}{2} v^8 + \cdots \right)$$

4.6 2D Ising Model: Low Temperature Expansion

For the low temperature expansion can be used, that the ground state $E_0 = -2NJ$ (all spins aligned) and the lower excited states give the dominating terms:

$$Z = \mathrm{Tr}(e^{-\beta H}) = W(E_0)e^{-\beta E_0} + W(E_1)e^{-\beta E_1} + W(E_2)e^{-\beta E_2} + \cdots$$

$$= e^{-\beta E_0}\left(1 + W(E_1)e^{-\beta \epsilon_1} + W(E_2)e^{-\beta \epsilon_2} + \cdots \right).$$

Here, $W(E_0) = 1$ and $\epsilon_i := E_i - E_0$ is used. A the first excited state, one spin is anti-aligned to all the others, hence $\epsilon_1 = 4 \cdot 2J$, with 4 nearest neighbors, and $W(E_1) = N$. For the second exited state, two connected spins flip together, yielding $\epsilon_2 = 6 \cdot 2J$, and $W(E_2) = 2N$. Therefore, the procedure is exactly the same as for the high temperature expansion and the result is very similar:

$$Z = u^N \left(1 + N u^4 + 2N u^6 + \frac{N(N-5)}{2} u^8 + \cdots \right), \quad u := e^{-2\beta J}.$$

5 Landau Theory

5.1 Free Energy

Suppose in general a Hamiltonian $H = H_0 - h\hat{m}$, where H_0 is the internal Hamiltonian of the system, h is an external field and $\hat{m}$ is the "response" operator. Then, the order parameter is $m = \langle\hat{m}\rangle$. The Gibbs free energy is

$$G = U - TS - hm, \qquad dG = -SdT - mdh,$$

where $U = \langle H_0 \rangle$. The free energy is

$$F = G + hm, \qquad dF = -SdT + hdm.$$

The order parameter and the external field are related by

$$m = -\frac{\partial G}{\partial h}, \qquad h = \frac{\partial F}{\partial m}.$$

If the order parameter is known, one can apply mean field theory and replace $\hat{m}$ in the Hamiltonian with its mean field average. For $h = 0$, it is $F = G$. Assuming $G(-m) = G(m)$ yields

$$G_0(m, T) = a + \frac{b}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6 + \cdots,$$

where $a, b, c, d, \dots$ are functions of T. For $h \neq 0$ it is $G_h(m, t) = -hm + G_0(m, t)$.

5.2 Phase Transitions

The state of a thermodynamics system is at the free energy minimum. At higher temperature it is assumed here that the free energy is symmetric in m.

By definition it is $m = 0$ for $T > T_c$ and G has its minimum at $m = 0$. Hence, for $T > T_c$ it is $a, b, c, d, \dots > 0$.

CONTINUOUS PHASE TRANSITIONS:

Consider now, that for $T < T_c$, it is $b < 0$ and $a, c, d, \dots > 0$. To be specific, let

$$b = b_0 \cdot (T - T_c) + \mathcal{O}((T - T_c)^2), \qquad b_0 > 0.$$

The minimum condition becomes

$$\frac{\partial G}{\partial m} = b_0(T - T_c)m + cm^3 + \mathcal{O}(m^5) = 0.$$

The solutions for $T \approx T_c$ (and hence small m) are $m_0 = 0$ and (note that $T < T_c$!)

$$m_\pm \approx \pm\sqrt{-\frac{b_0}{c}(T - T_c)} \sim |T - T_c|^\beta, \qquad \beta = \frac{1}{2}.$$

DISCONTINUOUS PHASE TRANSITIONS:

Consider now, that for $T < T_c$, it is $c < 0$ and $a, b, d, \dots > 0$. Let $\dot{m}$ be the zeroes and $\breve{m}$ be the extrema of $G_0 - a$. The zeroes are:

$$G_0 - a \approx \frac{b}{2}m^2 + \frac{c}{4}m^4 + \frac{d}{6}m^6 \overset{!}{=} 0$$

$$\implies \quad \dot{m}^2 \in \left\{0; 3/4d\left(-c \pm \sqrt{c^2 - 16db/3}\right)\right\}.$$

Those give at maximum five solutions for $\dot{m}$. The extrema are:

$$\frac{\partial G_0}{\partial m} = bm + cm^3 + dm^5 \overset{!}{=} 0$$

$$\implies \quad \breve{m}^2 \in \left\{0; 1/2d\left(-c \pm \sqrt{c^2 - 4bd}\right)\right\}.$$

Those give at maximum five solutions for $\breve{m}$ as well. However, there are four qualitatively different situations now (the graphs plot $G_0 - a$ versus m for different temperatures $T_1 > T_2 > T_3$):

T_1 has only one minima, hence it is

$$c^2 < 4bd.$$

T_2 has three minima, but only one zero, hence it is

$$4bd < c^2 < 16bd/3.$$

T_3 has three zeros, hence it is

$$16bd/3 < c^2.$$

The "main" critical temperature T_c is now reached for $c^2 = 16bd/3$, when the outer minima a lower than the inner minimum. However, the system may stay also for $T < T_c$ in the inner minimum (metastable). And, for growing T, it may stay in the outer minimum up to $T_c' > T_c$, which is found by $c^2 = 4bd$.
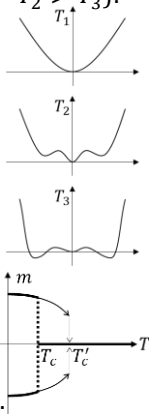
5.3 Latent Heat

Consider a system at $T = T_3$ (see bottom of 5.2). For growing temperature, the system will reach $T = T_c$, where $G_0 - a$ has exactly three zeros. Then, the system will jump from

$$\dot{m}_\pm = \pm\sqrt{-\frac{3c}{4d}} \qquad \text{to} \qquad \dot{m}_0 = 0,$$

which keeps the temperature at T_c, but increases the entropy and therefore needs the so-called "latent" heat

$$\Delta Q = T_c\Delta S = -T_c\left(\left.\frac{\partial G}{\partial T}\right|_{\dot{m}_0} - \left.\frac{\partial G}{\partial T}\right|_{\dot{m}_\pm}\right).$$

Since all coefficients are positive except for c, which changes sign at T_c', one can assume that $c \approx c_0(T - T_c')$ and the other coefficients are approximately constant at $T \approx T_c$. Thus, it is

$$\frac{\partial G}{\partial T} \equiv G' \approx a' + \frac{1}{2}b'm^2 + bmm' + \frac{1}{4}c'm^4 + cm^3m'$$

$$= bmm' + \frac{1}{4}c'm^4 + cm^3m'$$

and therefore (recalling $\dot{m}_0$ and $\dot{m}_\pm$ from above) it is

$$\Delta Q = T_c\Delta S = -T_c\left(\left.\frac{\partial G}{\partial T}\right|_{\dot{m}_0} - \left.\frac{\partial G}{\partial T}\right|_{\dot{m}_\pm}\right)$$

$$\approx T_c\left(bmm' + \frac{1}{4}c'm^4 + cm^3m'\right)\Big|_{\dot{m}_\pm}$$

$$= T_c\left(-\frac{3bc_0}{8d} + \frac{c_0}{4}\left(\frac{3c}{4d}\right)^2 + \frac{c_0}{2}\left(\frac{3c}{4d}\right)^2\right),$$

where it was used that

$$\dot{m}_\pm' = \pm\frac{\partial}{\partial T}\sqrt{-\frac{3c}{4d}} = \pm\frac{-\frac{3c_0}{4d}}{2\sqrt{-\frac{3c}{4d}}}.$$

5.4 Ginzburg-Landau Theory of Fluctuations

GINZBURG-LANDAU EQUATION:

To include the fluctuation into the mean field theory, the Landau theory is generalized to $m \to m(\vec{r})$. Hence, the free energy is

$$G[m(\vec{r}), T] = \int d^d r \left(-hm + a + \frac{b}{2}m^2 + \frac{c}{4}m^4 + \cdots + \frac{f}{2}(\nabla m)^2 \right),$$

where m, h are functions of $\vec{r}$ and a, b, c are functions of T. To take fluctuations into account, ∇m was introduced to the lowest order, which keeps G symmetrical w.r.t. m. The minimum of the free energy is determined by $\delta G = 0$ which gives

$$\delta G = \int d^d r \left(-h\,\delta m + bm\,\delta m + cm^3\,\delta m + \cdots - f\,\nabla^2 m\,\delta m \right) \overset{!}{=} 0,$$

where it was used that $\delta \nabla = \nabla \delta$ and by integration by parts it is $\int d^3 r\, \nabla m\, \nabla \delta m = -\int d^3 r\, \nabla^2 m\, \delta m$. Since the variation is arbitrary, this leads to the Ginzburg-Landau equation:

$$bm + cm^3 + \cdots - f\,\nabla^2 m = h.$$

DISSIPATION-FLUCTUATION RELATION:

Consider a weak field $h(\vec{r})$. The Hamiltonian can be written as

$$H = H_0 - \int d^d r\, h(\vec{r})\hat{m}(\vec{r}), \qquad m(\vec{r}) = \langle \hat{m}(\vec{r}) \rangle = \frac{\text{Tr}(\hat{m}(\vec{r})e^{-\beta H})}{\text{Tr}(e^{-\beta H})}.$$

Taylor expansion up to the leading order yields ($\hat{m}' := \hat{m}(\vec{r}')$)

$$m(\vec{r}) \approx \frac{\text{Tr}(\hat{m}e^{-\beta H_0}) + \text{Tr}(\hat{m}\beta \int d^d r'\, h'\hat{m}'e^{-\beta H_0})}{\underbrace{\text{Tr}(e^{-\beta H_0})}_{=Z_0} + \text{Tr}(\beta \int d^d r'\, h'\hat{m}'e^{-\beta H_0})}$$

$$= \frac{Z_0^{-1}\text{Tr}(\hat{m}e^{-\beta H_0}) + \beta \int d^d r'\, h' Z_0^{-1}\text{Tr}(\hat{m}\hat{m}'e^{-\beta H_0})}{1 + \beta \int d^d r'\, h' Z_0^{-1}\text{Tr}(\hat{m}'e^{-\beta H_0})}$$

$$= \frac{\langle \hat{m} \rangle_0 + \beta \int d^d r'\, h' \langle \hat{m}\hat{m}' \rangle_0}{1 + \beta \int d^d r'\, h' \langle \hat{m}' \rangle_0} \qquad \frac{1}{1+x} \approx 1 - x$$

$$\approx \langle \hat{m} \rangle_0 - \beta \int d^d r'\, h' \langle \hat{m} \rangle_0 \langle \hat{m}' \rangle_0 + \beta \int d^d r'\, h' \langle \hat{m}\hat{m}' \rangle_0 + \mathcal{O}(h^2),$$

where the mean $\langle \hat{m} \rangle_0$ is w.r.t. H_0 only. The fluctuation in m is

$$m - \langle \hat{m} \rangle_0 \approx \beta \int d^d r'\, h'(\langle \hat{m}\hat{m}' \rangle_0 - \langle \hat{m} \rangle_0 \langle \hat{m}' \rangle_0) = \beta \int d^d r'\, h'\, g',$$

where $g' \equiv g(\vec{r}, \vec{r}')$ is the correlation function (that is to say the fluctuation w.r.t. equilibrium without external perturbation). If $h(\vec{r}) = h_0 = \text{const.}$, the susceptibility (relative response) is

$$\chi(\vec{r}) = \frac{m(\vec{r}) - \langle \hat{m}(\vec{r}) \rangle_0}{h_0} = \beta \int d^d r'\, g(\vec{r}, \vec{r}'),$$

which is the exact and general "fluctuation-dissipation theorem".

POINT-LIKE PERTURBATION:

For $h = 0$, possible solutions of the Ginzburg-Landau eq. are

$$m_0 = \pm\sqrt{-b/c} \qquad \text{or} \qquad m_0 = 0 \quad \text{(for } b > 0\text{)}.$$

For $b \sim (T - T_c)$ it is $b > 0 \Leftrightarrow T > T_c$. Consider for a small h_0

$$h(\vec{r}) = h_0 \delta(\vec{r}).$$

Since h_0 is small, m can be written as a modification of m_0:

$$m(\vec{r}) = m_0 + \phi(\vec{r}).$$

Hence, the Ginzburg-Landau equation becomes

$$bm_0 + b\phi + cm_0^3 + 3cm_0^2\phi + \mathcal{O}(\phi^2) + \cdots - f\,\nabla^2\phi$$
$$\approx \alpha\phi - f\,\nabla^2\phi = h_0\delta(\vec{r}),$$

where $\alpha := b + 3cm_0^2 \in \{b, -2b\}$, which depends on if $b \lessgtr 0$. Multipliying by $e^{-i\vec{k}\vec{r}}$ and integration over d dimensions yields

$$\alpha \int d^d r\, e^{-i\vec{k}\vec{r}}\phi(\vec{r}) - f \int d^d r\, e^{-i\vec{k}\vec{r}}\nabla^2\phi(\vec{r}) = h_0 \int d^d r\, e^{-i\vec{k}\vec{r}}\delta(\vec{r})$$

$$\Leftrightarrow \quad \alpha\tilde{\phi}(\vec{k}) + f\vec{k}^2\tilde{\phi}(\vec{k}) = h_0 \quad \Leftrightarrow \quad \tilde{\phi}(\vec{k}) = h_0/(\alpha + f\vec{k}^2),$$

where the second term was integrated by parts twice and the Fourier transformed $\tilde{\phi}$ of ϕ was used. Then, the solution is:

$$\phi(\vec{r}) = \int d^d k\, \tilde{\phi}(\vec{k})e^{i\vec{k}\vec{r}} = \frac{h_0}{4\pi f}\frac{e^{-r/\xi}}{r^{d-2}}, \qquad \xi = \sqrt{f/|\alpha|},$$

where ξ is the "correlation length". For $b(T) \sim (T - T_c)$, it is

$$\xi \sim |T - T_c|^{-\nu}, \qquad \nu = 1/2,$$

where ν is another critical exponent. The susceptibility is

$$\chi(\vec{r}) = \frac{\phi(\vec{r})}{h_0} = \frac{m - \langle \hat{m} \rangle_0}{h_0} = \beta \int d^d r'\, \delta(\vec{r}')g' = \beta g(\vec{r}, \vec{0}).$$

5.5 Validity of the Landau Theory

From 5.4, it is ($b \sim (T - T_c)$):

$$g(\vec{r}, 0) \sim \phi(\vec{r}) \sim \frac{e^{-r/\xi}}{r^{d-2}},$$

$$m_0 = \pm\sqrt{-\frac{b}{c}} \sim |T - T_c|^\beta, \qquad \xi \sim |T - T_c|^{-\nu},$$

where $\beta = \nu = 1/2$. For the mean field theory to be valid, the fluctuations should be much smaller than the mean order parameter:

$$1 \overset{!}{\gg} \frac{\int_{r<\xi} d^d r\, g(\vec{r}, 0)}{\int_{r<\xi} d^d r\, m_0^2} \sim \frac{\int_{r<\xi} r^{d-1}dr\, e^{-r/\xi}r^{2-d}}{|T - T_c|^{2\beta}\int_{r<\xi} d^d r\, 1} = \frac{\int_{r<\xi} dr\, e^{-r/\xi}r}{|T - T_c|^{2\beta}\xi^d}$$

$$= \frac{\xi^2 \int_{x<1} dx\, e^{-x}x}{|T - T_c|^{2\beta}\xi^d} \sim \frac{\xi^{2-d}}{|T - T_c|^{2\beta}} \sim \frac{|T - T_c|^{-2\nu+d\nu}}{|T - T_c|^{2\beta}},$$

where the substitution $x := r/\xi$ was used. This yields

$$1 \overset{!}{\gg} |T - T_c|^{-2\nu+d\nu-2\beta} \quad \Leftrightarrow \quad -2\nu + d\nu - 2\beta > 0 \quad \Leftrightarrow \quad d > 4$$

(near the critical point). Since it is also a valid theory for $d = 4.00001$, it is expected to be also a good theory for $d \geq 4$. That is to say: Recall, that the fluctuation a biggest near the critical point. Hence, for $d < 3$, the mean field theory might still be valid for $T \not\approx T_c$. It depends on the system, how close to the critical temperature the mean field theory is a good theory and for some systems, it is closer than the accuracy of measurement.

6 The Widom Scaling Hypothesis

6.1 Relations between critical exponents

Consider the critical exponents for the following examples. Here, it is $t := |T - T_c|$ and moreover $\dot{G} := \partial_t G$ as well as $G' := \partial_h G$.

	Definition	MFT	2D Ising	3D Ising
α	$c_H = -T\ddot{G} \sim |t|^{-\alpha}$	0	0	0.1096
β	$m = -G' \sim |t|^{\beta}$	1/2	1/8	0.32653
γ	$\chi = -G'' \sim |t|^{-\gamma}$	1	7/4	1.2373
δ	$m \sim h^{1/\delta}$	3	15	4.7893
η	$g \sim e^{-r/\xi} r^{-d+2-\eta}$	0	1/4	0.03639
ν	$\xi \sim |t|^{-\nu}$	1/2	1	0.63012

Firstly, note that the mean field theory (MFT) is much more valid for the 3D system than for the 2D system. Secondly, note that it is always:

→ $\quad \alpha + 2\beta + \gamma = 2 \qquad$ (Rushbrooke inequality)
→ $\quad \alpha + \beta(\delta + 1) = 2$
→ $\quad \gamma = \nu(2 - \eta)$
→ $\quad \alpha = 2 - d\nu \qquad$ (hyper-scaling law)

The hyper-scaling law contains the dimension d and is therefore not valid for the mean field theory, which is independent of the dimension.

6.2 The Scaling Hypothesis

Since there are four relating equations for the six critical exponents, only two of them are independent. Therefore, there should be an equation of state, which depends only on two parameters, for example temperature $t = (T - T_c)/T_c$ and the external field $h = (H - H_c)/kT_c$. It is

$$h \sim m^\delta, \qquad t \sim m^{1/\beta}.$$

If now m is scaled by a factor l like $m' = lm$, it follows

$$h' = l^\delta h, \qquad t' = l^{1/\beta} t.$$

From 5.1 it is known that

$$m = -\frac{\partial G(t,h)}{\partial h} \implies -l\frac{\partial G(t,h)}{\partial h} = lm = -\frac{\partial G(l^{1/\beta}t, l^\delta h)}{\partial(l^\delta h)}$$

$$\iff \quad G(t,h) = l^{-\delta-1} G(l^{1/\beta}t, l^\delta h),$$

which can be written in a more general form

$$G(t,h) = \lambda G(\lambda^s t, \lambda^r h)$$

by using $\lambda := l^{-\delta-1}, s = -1/\beta(1+\delta), r = -\delta/(1+\delta)$. The point is that the function $G(x,y)$ is (for $T \approx T_c$) on the left and right hand side the same, only the scaling is different.

The critical exponents can now be given in terms of s and r. First, consider the order parameter:

$$m(t,h) = -\frac{\partial G(t,h)}{\partial h} = -\frac{\partial \lambda G(\lambda^s t, \lambda^r h)}{\partial h} = -\lambda^r \frac{\partial \lambda G(\lambda^s t, \lambda^r h)}{\partial(\lambda^r h)}$$

$$= -\lambda^{r+1} \frac{\partial G(\lambda^s t, \lambda^r h)}{\partial(\lambda^r h)} = \lambda^{r+1} m(\lambda^s t, \lambda^r h)$$

Similarly,

$$\chi(t,h) = -\frac{\partial^2 G(t,h)}{\partial h^2} = -\lambda^{2r} \frac{\partial^2 \lambda G(\lambda^s t, \lambda^r h)}{\partial(\lambda^r h)^2} = \lambda^{2r+1} \chi(\lambda^s t, \lambda^r h),$$

$$c_H = -t\frac{\partial^2 G}{\partial t^2} = -t\lambda^{2s} \frac{\partial^2 \lambda G(\lambda^s t, \lambda^r h)}{\partial(\lambda^s t)^2} = \lambda^{2s+1} c_H(\lambda^s t, \lambda^r h).$$

Taking, for example, $\lambda = |t|^{-1/s}$ at $h = 0$ yields

$$m(t < 0,0) = |t|^{-(r+1)/s} m(-1,0),$$
$$\chi(\pm|t|,0) = |t|^{-(2r+1)/s} \chi(\pm 1,0),$$
$$c_H(\pm|t|,0) = |t|^{-(2s+1)/s} c_H(\pm 1,0)$$

and if $\lambda = |h|^{-1/r}$ at $t = 0$,

$$m(0, \pm|h|) = |h|^{-(r+1)/r} m(0, \pm 1).$$

Hence, it is

$$\alpha_\pm = \frac{2s+1}{s}, \quad \beta = -\frac{r+1}{s}, \quad \gamma_\pm = \frac{2r+1}{s}, \quad \delta = -\frac{r}{r+1}.$$

Those results satisfy

$$\alpha + 2\beta + \gamma = 2, \qquad \beta(\delta - 1) = \gamma.$$

6.3 Kadanoff Blocks

Consider a d-dimensional Ising model with free energy $G(t,h)$ near the critical point. For $L \ll \xi$, ξ being the correlation length, one can take a block of L^d spins as if it were just one spin. Near the critical point, the free energy in terms of the blocks has the same form as the original one. However, the new correlation length $\xi_L = \xi/L$ now looks shorter and the distance to the critical point, measured by t, h looks larger:

$$t_L = L^y t, \qquad h_L = L^x h.$$

The free energy of a block of spins is lager as of only one spin:

$$G_L \equiv G(L^y t, L^x h) = L^d G(t,h).$$

Comparison to $G(t,h) = \lambda G(\lambda^s t, \lambda^r h)$ (see 6.2) yields:

$$\lambda = L^{-d}, \qquad y = -sd, \qquad x = -rd.$$

Let $h = 0$ and $L = |t|^{-1/y}$ yields $\lambda = |t|^{d/y}$ and thus, using 6.2:

$$c_H(t,0) = \lambda^{2s+1} c_H(\lambda^s t, \lambda^r 0) = |t|^{-2+d/y} c_H(\pm 1,0),$$
$$\xi(t,0) = L\xi_L = L\xi(\lambda^s t, \lambda^r 0) = |t|^{-1/y} \xi(\pm 1,0).$$

This yields $\nu = 1/y$ and $\alpha = 2 - d/y$ and hence the hyper-scaling law:

$$\alpha = 2 - d/y = 2 - d\nu.$$

7 Renormalization Group Theory

7.1 Fixed Points, Conducting Pearls

INTRODUCTORY EXAMPLE, FIX POINTS:

Consider a d-dimensional box with made up of N tightly packed pearls, each of which is conducting with probability P and isolating with probability $1 - P$. If $P > P_c$, the whole box is conducting and else isolating for $N \to \infty$. For $d = 1$, it is $P_c = 1$, hence all pearls have to be conducting and for any $P < 1$ the chain is insulating for $N \to \infty$, what can be shown by renormalization:

The probability of a block of two neighbouring pearls to conduct is
$$P_1 = R(P) = P^2.$$
The probability of a super block made up of two neighbouring blocks to conduct is
$$P_2 = R(P_1) = P_1^2.$$
For the n-order super block it is
$$P_n = R(P_{n-1}) = P_{n-1}^2 = P^{(2^n)}, \qquad P_0 = P.$$
The two values $P^* = 0$ and $P^* = 1$ are interesting, since
$$P^* = R(P^*).$$
Such points are called *fixed points*. For a $P \neq P^*$, the renormalized value P_n would be farther and farther to $P^* = 1$ and closer and closer to $P^* = 0$ for increasing n. Thus, $P^* = 0$ is called a *stable fix point* and $P^* = 1$ an *unstable fix point*. In general, an unstable fixed point corresponds to a critical point.

DETERMINE FIX POINTS AND THEIR STABILITY:

Blocking always b neighbouring pearls, the renormalized conducting probability is
$$R_b(P) = P^b$$
and the fix points are determined by the equation
$$P^* = R_b(P^*).$$
The solutions are, again, $P^* = 0, 1$. To see if a fix point is stable, consider a small deviation from the fixed points
$$\delta P := P - P^*,$$
which, after renormalization, is
$$\delta R_b(P^*) = R_b(P^* - \delta P) - R_b(P^*) = \left.\frac{dR_b(P)}{dP}\right|_{P=P^*} \delta P =: \lambda_b \, \delta P,$$
which defines the λ_b. Now, the fix point is stable if $\lambda_b < 1$ and unstable if $\lambda_b > 1$. In this case, it should be $b \geq 2$ and hence
$$\lambda_b = \left.\frac{dR_b(P)}{dP}\right|_{P=P^*} = bP^{*b-1} = \begin{cases} 0 < 1, & \text{for } P^* = 0 \Rightarrow \text{stable,} \\ b > 1, & \text{for } P^* = 1 \Rightarrow \text{unstable.} \end{cases}$$
Here, P is farther and farther away from the critical point $P_c = 1$ and thus it is called *relevant*; otherwise it is called *irrelevant*.

BEHAVIOUR NEAR THE CRITICAL POINT $P_c = 1$:

The correlation length ξ is the average length of conducting pearls. Under renormalization, it should scale as
$$\xi'(P) := \xi\big(R_b(P)\big) \stackrel{!}{=} \xi(P)/b$$
and the corresponding critical exponent is defined by
$$\xi \sim |P - P_c|^{-\nu}.$$
Under renormalization, it is (using $\lambda_b = bP^{b-1}|_{P=P_c=1} = b$):
$$\underbrace{P' - P_c}_{=\delta R_b(P)} = \lambda_b \underbrace{(P - P_c)}_{=\delta P} + \mathcal{O}(|P - P_c|^2)$$
Hence, it is
$$b = \frac{\xi}{\xi'} = \frac{|P - P_c|^{-\nu}}{|P' - P_c|^{-\nu}} = \lambda_b^\nu \quad \Leftrightarrow \quad \nu = \frac{\ln b}{\ln \lambda_b} = \frac{\ln b}{\ln\big(bP^{b-1}|_{P_c}\big)} = 1.$$

7.2 1D Ising Model: Renormalized Partition Function

Consider the 1D Ising model with periodic boundary conditions in terms of the dimensionless Hamiltonian
$$H_0 = -\beta H = K_0 \sum_{j=1}^N \sigma_j \sigma_{j+1} + h_0 \sum_{j=1}^N \sigma_j, \qquad K_0 := \frac{J}{kT}, \quad h_0 := \frac{h}{kT}.$$
The partition function is
$$Z(N, K_0, h_0) = \sum_{\sigma_{1,2,\dots,N}=\pm 1} e^{H_0} = \sum_{\sigma_2,\sigma_4,\dots} \sum_{\sigma_1,\sigma_3,\dots} \prod_{j=1}^N e^{K_0 \sigma_j \sigma_{j+1} + h_0 \sigma_j}$$
$$= \sum_{\sigma_2,\sigma_4,\dots} \prod_{j=1,3,\dots} \sum_{\sigma_j=\pm 1} e^{K_0(\sigma_{j-1}\sigma_j + \sigma_j\sigma_{j+1}) + h_0(\sigma_{j-1} + 2\sigma_j + \sigma_{j+1})/2}.$$
Obviously, because there is only next-nearest interaction, it is possible to separate the sums over only the odd-numbered spins, but not all the sums due to the coupling $\sigma_j\sigma_{j+1}$. It is
$$\sum_{\sigma_j=\pm 1} e^{K_0(\sigma_{j-1}\sigma_j + \sigma_j\sigma_{j+1}) + h_0(\sigma_{j-1} + 2\sigma_j + \sigma_{j+1})/2}$$
$$= e^{-K_0(\sigma_{j-1}+\sigma_{j+1}) + h_0(\sigma_{j-1} - 2 + \sigma_{j+1})/2}$$
$$\quad + e^{K_0(\sigma_{j-1}+\sigma_{j+1}) + h_0(\sigma_{j-1} + 2 + \sigma_{j+1})/2}$$
$$= e^{h_0(\sigma_{j-1}+\sigma_{j+1})/2} \left(e^{-K_0(\sigma_{j-1}+\sigma_{j+1}) - h_0} + e^{K_0(\sigma_{j-1}+\sigma_{j+1}) + h_0}\right)$$
$$= 2e^{h_0(\sigma_{j-1}+\sigma_{j+1})/2} \cosh\big(K_0(\sigma_{j-1} + \sigma_{j+1}) + h_0\big).$$
Using $\cosh x \approx 1 + x^2/2$ yields
$$2\cosh\big(K_0(\sigma_{j-1} + \sigma_{j+1}) + h_0\big) \approx 2 + \big(K_0(\sigma_{j-1} + \sigma_{j+1}) + h_0\big)^2$$
$$= 2 + K_0^2(\sigma_{j-1} + \sigma_{j+1})^2 + 2K_0 h_0(\sigma_{j-1} + \sigma_{j+1}) + h_0^2$$
$$= 2 + h_0^2 + 2K_0^2 + 2K_0^2 \sigma_{j-1}\sigma_{j+1} + 2K_0 h_0(\sigma_{j-1} + \sigma_{j+1})$$
$$\stackrel{!}{=} \exp\big(-2g + K_1\sigma_{j-1}\sigma_{j+1} + (h_1 - h_0)(\sigma_{j-1} + \sigma_{j+1})/2\big).$$
Considering the four possible combinations of values of $\sigma_{j-1}, \sigma_{j+1}$ separately, this equation defines g, K_1, h_1 as
$$g(K_0, h_0) = -\frac{\ln(16 \cosh(h_0 + 2K_0) \cosh^2(h_0) \cosh(h_0 - 2K_0))}{8}$$
$$R_K(K_0, h_0) := K_1 = \frac{1}{4} \ln \frac{\cosh(2K_0 + h_0) \cosh(2K_0 - h_0)}{\cosh^2(h_0)}$$
$$R_h(K_0, h_0) := h_1(K_0, h_0) = h_0 + \frac{1}{2} \ln \frac{\cosh(2K_0 + h_0)}{\cosh(2K_0 - h_0)}.$$
Those are called *renormalization flow equations.* Thereby, the partition function is
$$Z = \sum_{\sigma_2,\sigma_4,\dots} \prod_{j=1,3,\dots} 2e^{h_0(\sigma_{j-1}+\sigma_{j+1})/2} \cosh\big(K_0(\sigma_{j-1} + \sigma_{j+1}) + h_0\big)$$
$$= \sum_{\sigma_2,\sigma_4,\dots} \prod_{j=1,3,\dots} e^{h_0(\sigma_{j-1}+\sigma_{j+1})/2} e^{-2g + K_1\sigma_{j-1}\sigma_{j+1} + (h_1 - h_0)(\sigma_{j-1}+\sigma_{j+1})/2}$$
$$= e^{-Ng} \sum_{\sigma_2,\sigma_4,\dots} \prod_{j=2,4,\dots} e^{K_1\sigma_j\sigma_{j+2} + h_1\sigma_j}$$
$$= e^{-Ng} \sum_{\sigma_2,\sigma_4,\dots} \prod_{j=1}^{N/2} e^{K_1\sigma_{2j}\sigma_{2j+2} + h_1\sigma_{2j}}.$$
Obviously, it is
$$Z(N, K_0, h_0) = e^{-Ng(K_0,h_0)} Z(N/2, K_1, h_1)$$
$$= e^{-Ng(K_0,h_0)} e^{-(N/2)g(K_1,h_1)} Z(N/4, K_2, h_2)$$
$$= e^{-N \sum_{k=0}^n 2^{-k} g(K_k,h_k)} Z(2^{-n-1}N, K_n, h_n)$$
$$\xrightarrow[n\to\infty]{} e^{-N \sum_{k=0}^\infty 2^{-k} g(K_k,h_k)},$$
with the recursion relations for the parameters
$$K_{k+1} = R_K(K_k, h_k), \qquad h_{k+1} = R_h(K_k, h_k).$$

7.3 1D Ising Model: Free Energy

The free energy per spin is, for $n \to \infty$,

$$f(K_0, h_0) = -\frac{kT}{N} \ln Z = kT \sum_{k=0}^{\infty} 2^{-k} g(K_k, h_k),$$

which can be shown to satisfy

$$f(K_0, h_0) = kT g(K_0, h_0) + 2^{-1} f(K_1, h_1)$$
$$= -K_0 kT - kT \ln \left(\cosh h_0 + \sqrt{e^{-4K_0} + \sinh^2 h_0} \right).$$

SPECIAL CASE $K_0 = 0$:
For the special case $K_0 = 0$, it is (from 7.2)

$$R_K(0, h_0) = 0, \qquad R_h(0, h_0) = h_0,$$

thus $(0, h_0)$ is a fixed point. The free energy becomes

$$f(0, h_0) = -kT \ln(2 \cosh h_0) = -kT \ln(e^{h_0} + e^{-h_0}).$$

SPECIAL CASE $h_0 = 0$:
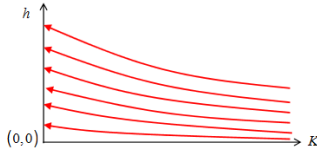For the special case $h_0 = 0$, it is (from 7.2)

$$R_K(K_0, 0) = 2^{-1} \ln \cosh(2K_0), \qquad R_h(K_0, 0) = 0.$$

The free energy is

$$f(K_0, 0) = -K_0 kT - kT \ln(1 + e^{-2K_0})$$
$$= -K_0 kT - kT \ln\left(e^{-K_0}(e^{K_0} + e^{-K_0})\right) = -kT \ln(2 \cosh K_0).$$

7.4 1D Ising Model: Renormalization Flow

From the renormalization flow equation, for some starting point (h_0, K_0), the flow is shown in the following diagram:

Recall from 7.3 the renormalization flow equations for $h_0 = 0$:

$$K' := R_K(K_0, 0) = \ln \cosh(2K_0)/2, \qquad h' := R_h(K_0, 0) = 0.$$

From the figure it is obvious that $K^* = 0$ is a fixed point, for which (from 7.2)

$$g(K^* = 0, 0) = -(\ln 2)/2.$$

For a big enough $k = k_0$, the renormalized coupling is close enough to the fixed point to replace $g(K_n, 0)$ with $g(K^*, 0)$ and hence, the free energy is

$$f(K_0, h_0) \approx kT \sum_{k=0}^{k_0} 2^{-k} g(K_k, h_k) + kT g(K^*, 0)$$

$$= kT \sum_{k=0}^{k_0} 2^{-k} g(K_k, 0) - \frac{kT}{2} \ln 2.$$

The fixed point $(0,0)$ is stable, since

$$\left. \frac{dR_K(K_0, 0)}{dK_0} \right|_{K_0 = K^* = 0} = \frac{1}{2} \frac{d}{dK_0} \ln \cosh(2K_0) \Big|_{K_0 = K^* = 0} = 0 < 1.$$

Another (unstable) fixed point is $(K^*, h^*) = (\infty, 0)$, which corresponds to $T = 0$ and is actually the only critical point of the system. The flow equation near that point are (from 7.2)

$$K' := \frac{1}{4} \ln \frac{\cosh(2K + h) \cosh(2K - h)}{\cosh^2(h)} \approx \frac{1}{2} \ln \cosh(2K)$$

$$= \frac{1}{2} \ln \left(\frac{1}{2}(e^{2K} + e^{-2K}) \right) \approx K - \frac{1}{2} \ln 2,$$

$$h' := h + \frac{1}{2} \ln \frac{\cosh(2K + h)}{\cosh(2K - h)} \approx h + h \tanh(2K) \approx 2h = b^{x_h} h,$$

where in both flow equations at the first $\approx$-sign a Taylor expansion at $h \approx 0$ was conducted. x_h is defined by this equation. The infinite critical parameter is not so convenient; using $\tau := e^{-pK}, p > 0$, yields (which defines x_τ)

$$-(\ln \tau')/p = -(\ln \tau)/p - (\ln 2)/2 \quad \Leftrightarrow \quad \tau' = 2^{p/2} \tau = b^{x_\tau} \tau.$$

Thus, the free energy becomes

$$f(h, \tau) = 2^{-1} f(2h, 2^{p/2} \tau) = 2^{-k} f(2^k h, 2^{kp/2} \tau)$$
$$= L^{-1} f(Lh, L^{p/2} \tau).$$

In the same way as in 6, this yields

$$\alpha = 2 - 2/p, \quad \beta = 0, \quad \gamma = 2/p, \quad \delta = \infty, \quad \nu = 2/p, \quad \eta = 1.$$

7.5 General Renormalization Group Theory

RENORMALIZATION:
For a general formulation, consider a dimensionless Hamiltonian

$$H = -\beta \widetilde{H} = \sum_{\alpha=1}^{n} k_\alpha \psi_\alpha(\{\sigma_i\}),$$

where σ_i is an operator corresponding to a particle (or spin) at position i. The partition function is, using $K = \{k_i\}$,

$$Z(N, K) = \text{Tr}_{\{\sigma_i\}}(e^{H(N,K)}).$$

Divide the d-dimensional system into blocks of size b^d and label the blocks by indices I and the spins within one block with indices m, such that $i = (I, m)$. The partition function is now

$$Z(N, K) = \text{Tr}_{\{\sigma_I\}} \left(e^{-Ng(K)} e^{H'(N/b^d, K')} \right) = e^{-Ng(K)} Z(N/b^d, K'),$$

where

$$H'(N/b^d, K') = \sum_{\alpha=1}^{n} k_\alpha' \psi_\alpha(\{\sigma_I\}), \qquad f(K) = g(K) + b^{-d} f(K')$$

and the k_α' are given by the renormalization flow equations

$$k_\alpha' = R_\alpha(k_1, k_2, \dots, k_n) \quad \Leftrightarrow \quad K' = R(K).$$
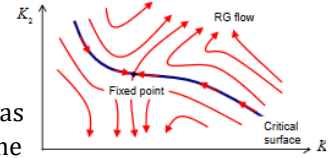
FIXED POINTS, CRITICAL SURFACE:
The arrows from K to $R(K)$ to $R(R(K))$ form a flow in the parameter space. Moreover, fix points K^* are defined as

$$K^* = R(K^*).$$

Critical points K_c in general form a surface in the parameter space. The flow never crosses a critical surface, as argued now: At the critical surface, the correlation length ξ is infinite; close to the surface ξ is big but finite. The correlation length scales like $\xi' = b^{-1}\xi < \xi$, therefore, renormalized parameters flow *away* from the critical surface (a disordered never looks ordered on a larger scale). Right *on* the surface, $\xi' = \xi = \infty$ is unchanged and hence K_c' is also still on the surface and usually flows to a fixed point K_c^*, which is a saddle point on the surface. All critical points flowing to the same fixed point have the same critical exponents, since the singularity part of the free energy is unchanged under renormalization.

CRITICAL BEHAVIOUR:
Consider parameters near the critical fixed point and their flow equations

$$k_\alpha = k_\alpha^* + dk_\alpha, \qquad k_\alpha' = R_\alpha(k_1, k_2, \dots).$$

The distance from the critical fixed point is after renormalization

$$dk_\alpha' = \sum_\beta \left. \frac{\partial R_\alpha(K)}{\partial k_\beta} \right|_{K = K^*} dk_\beta = M_{\alpha\beta} dk_\beta,$$

which defines the matrix $M_{\alpha\beta}$. Also, define a diagonalizing matrix C such that

$$CMC^{-1} = \text{diag}(\lambda_1, \dots, \lambda_n) \Leftrightarrow CM = \text{diag}(\lambda_1, \dots, \lambda_n)C$$

and also $du_\gamma := C_{\gamma\alpha} dk_\alpha$ such that

$$du_\gamma' = C_{\gamma\alpha} dk_\alpha' = C_{\gamma\alpha} M_{\alpha\beta} dk_\beta = \left(\mathbb{I}\vec{\lambda}C \right)_{\gamma\beta} dk_\beta = \lambda_\gamma \delta_{\alpha\gamma} C_{\alpha\beta} dk_\beta$$
$$= \lambda_\gamma \delta_{\alpha\gamma} du_\alpha = \lambda_\gamma du_\gamma$$

(there are sums over double indices *except for γ*!). Now,
for $|\lambda_\gamma| < 1$, u_γ is "irrelevant" (flows into K_c^*),
for $|\lambda_\gamma| > 1$, u_γ is "relevant" (flows away from K_c^*),
for $|\lambda_\gamma| = 1$, u_γ is "marginal" (determined by higher orders).
Taking $\lambda_\gamma = b^{x_\gamma}$ (which defines x_γ), the correlation length scales for k repeated renormalizations

$$\xi(u_1, \dots, u_n) = b^k \xi(b^{kx_1}u_1, \dots, b^{kx_n}u_n).$$

Similarly, the singularity part of the free energy scales like

$$f_s(u_1, \dots, u_n) = b^{-dk} f_s(b^{kx_1}u_1, \dots, b^{kx_n}u_n),$$

which is just the scaling hypothesis. For large k, the irrelevant parameters will vanish and only relevant parameters will be left:

$$k \gg 1: \qquad f_s(u_1, \dots, u_n) = b^{-dk} f_s(b^{kx_1}u_1, b^{kx_2}u_2, \dots, 0, 0, \dots).$$

As in 6, the critical exponents can be obtained from here.

8 Topological Phase Transitions

8.1 Classical XY-Model

Consider the Hamiltonian

$$H = -J \sum_{\langle ij \rangle} \vec{s}_i \vec{s}_j = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \approx -J \sum_{\langle ij \rangle} \left(1 - \frac{1}{2}\phi_{ij}^2\right),$$

where $\vec{s}_i$ are vectors in a 2D space with $|s_i| = 1$ on a d-dimensional square lattice with lattice constant a. Hence, they can only rotate and are fully described by angles ϕ_i. Above, $\vec{s}_i \vec{s}_j = |\vec{s}_i||\vec{s}_j|\cos(\phi_i - \phi_j) = \cos(\phi_i - \phi_j)$ and $\phi_{ij} := \phi_i - \phi_j \ll 1$ was used. Now, the ϕ_i can be diagonalized by Fourier transformation

$$\phi_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \varphi_{\vec{k}} e^{i\vec{k}\vec{r}_i},$$

where $\vec{r}_i$ is the position of the spin with angle ϕ_i. Using this, the Hamiltonian (without the not interesting constant term) is

$$H \approx \frac{J}{2} \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 = \frac{J}{2N} \sum_{\langle ij \rangle} \left(\sum_{\vec{k}} \varphi_{\vec{k}} e^{i\vec{k}\vec{r}_i} - \sum_{\vec{k}} \varphi_{\vec{k}} e^{i\vec{k}\vec{r}_j} \right)^2$$

$$= \frac{J}{2N} \sum_{\langle ij \rangle} \left(\sum_{\vec{k}_1} \varphi_{\vec{k}_1} e^{i\vec{k}_1 \vec{r}_i} \sum_{\vec{k}_2} \varphi_{\vec{k}_2} e^{i\vec{k}_2 \vec{r}_i} \right.$$

$$\left. - 2 \sum_{\vec{k}_1} \varphi_{\vec{k}_1} e^{i\vec{k}_1 \vec{r}_i} \sum_{\vec{k}_2} \varphi_{\vec{k}_2} e^{i\vec{k}_2 \vec{r}_j} + \sum_{\vec{k}_1} \varphi_{\vec{k}_1} e^{i\vec{k}_1 \vec{r}_j} \sum_{\vec{k}_2} \varphi_{\vec{k}_2} e^{i\vec{k}_2 \vec{r}_j} \right)$$

$$= \frac{J}{N} \sum_{\langle ij \rangle} \sum_{\vec{k}_1, \vec{k}_2} \varphi_{\vec{k}_1} \varphi_{\vec{k}_2} \left(e^{i\vec{k}_1 \vec{r}_i + i\vec{k}_2 \vec{r}_i} - e^{i\vec{k}_1 \vec{r}_i + i\vec{k}_2 \vec{r}_j} \right)$$

$$= \frac{J}{N} \sum_{\langle ij \rangle} \sum_{\vec{k}_1, \vec{k}_2} \varphi_{\vec{k}_1} \varphi_{\vec{k}_2} \delta(\vec{k}_1 + \vec{k}_2) \left(1 - e^{i\vec{k}_1 \vec{r}_i + i\vec{k}_2 \vec{r}_j}\right)$$

$$= J \sum_{\vec{k}} \varphi_{\vec{k}} \varphi_{-\vec{k}} \left(q - \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} \right) \right)$$

$$= J \sum_{\vec{k}} \varphi_{\vec{k}} \varphi_{-\vec{k}} \left(q - 2(\cos k_x a + \cos k_y a) \right) = \sum_{\vec{k}} |\varphi_{\vec{k}}|^2 E(\vec{k}),$$

where q is the number of nearest neighbours and the energy is (in the lecture notes, there is an additional factor $1/2$ and I don't know where it comes from):

$$E(\vec{k}) = J(q - 2\cos k_x a - 2\cos k_y a)$$

$$\approx J\left(q - 2\left(1 - \frac{1}{2}(k_x a)^2\right) - 2\left(1 - \frac{1}{2}(k_y a)^2\right) \right)$$

$$= J(q - 4 + \vec{k}^2 a^2) = Ja^2 \vec{k}^2.$$

The last equation is for a 2D square lattice ($q = 4$). Thus, the partition function is

$$Z = \text{Tr}(e^{-\beta H}) = \prod_{\vec{k}} \int d\varphi_{\vec{k}}^* d\varphi_{\vec{k}} e^{-\beta E \varphi_{\vec{k}}^* \varphi_{\vec{k}}}$$

and hence the mean values are

$$\langle \varphi_{\vec{k}} \rangle = \frac{1}{Z} \text{Tr}(e^{-\beta H} \varphi_{\vec{k}}) = \frac{1}{Z} \prod_{\vec{k}'} \int d\varphi_{\vec{k}'}^* d\varphi_{\vec{k}'} e^{-\beta E |\varphi_{\vec{k}'}|^2} \varphi_{\vec{k}}$$

$$= \left(\int d\varphi_{\vec{k}}^* d\varphi_{\vec{k}} e^{-\beta E |\varphi_{\vec{k}}|^2} \varphi_{\vec{k}} \right) / \left(\int d\varphi_{\vec{k}}^* d\varphi_{\vec{k}} e^{-\beta E |\varphi_{\vec{k}}|^2} \right) = 0,$$

since it is the integration over a product of even and odd function. Similarly it is

$$\langle \varphi_{\vec{k}}^* \varphi_{\vec{k}} \rangle = \left(\int d\varphi_{\vec{k}}^* d\varphi_{\vec{k}} e^{-\beta E |\varphi_{\vec{k}'}|^2} |\varphi_{\vec{k}}|^2 \right) / \left(\int d\varphi_{\vec{k}}^* d\varphi_{\vec{k}} e^{-\beta E |\varphi_{\vec{k}'}|^2} \right)$$

$$= \frac{1}{2} \sqrt{\frac{\pi}{(\beta E)^3}} \cdot \sqrt{\frac{\beta E}{\pi}} = \frac{1}{2\beta E}.$$

8.2 Correlation

The correlation function is given by

$$g(\vec{r}_i - \vec{r}_j) = \langle (\vec{s}_i - \langle \vec{s}_i \rangle)(\vec{s}_j - \langle \vec{s}_j \rangle) \rangle = \langle \vec{s}_i \vec{s}_j \rangle,$$

since it can be shown that the order parameter is zero: $m = \langle s_i \rangle = 0$. Hence, consider only ($\phi_{i0} := \phi_i - \phi_0$):

$$G(\vec{r}_i) := \langle s_i s_0 \rangle = \langle \cos(\phi_i - \phi_0) \rangle = \text{Re}\langle e^{i\phi_{i0}} \rangle$$

$$= \text{Re}\left(\sum_{n=0}^{\infty} \frac{(-1)^n \langle \phi_{i0}^{2n} \rangle}{(2n)!} + i \sum_{n=0}^{\infty} \frac{(-1)^n \langle \phi_{i0}^{2n+1} \rangle}{(2n+1)!} \right)$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \langle \phi_{i0}^{2n} \rangle = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} (2n-1)!! \langle \phi_{i0}^2 \rangle^n$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{2^n n!} \langle \phi_{i0}^2 \rangle^n = e^{-\langle (\phi_i - \phi_0)^2 \rangle / 2},$$

where Wick's Theorem (for $\phi_a := \phi_i - \phi_0$)

$$\langle \phi_a \phi_b \phi_c \phi_d \cdots \rangle = \langle \phi_a \phi_b \rangle \langle \phi_c \phi_d \rangle \cdots + \langle \phi_a \phi_c \rangle \langle \phi_b \phi_d \rangle \cdots + \text{all pairs}$$

$$\implies \langle \phi_a^m \rangle = \langle \phi_a^2 \rangle^{m/2} + \langle \phi_a^2 \rangle^{m/2} + \cdots = (m-1)!! \langle \phi_a^2 \rangle^{m/2}$$

was used. By a similar same derivation and the energy $E = Ja^2 \vec{k}^2$ from 8.1 it is, assuming $\vec{r}_0 = 0$ (again, a factor 2 is missing here compared to lecture notes):

$$\langle (\phi_i - \phi_0)^2 \rangle = \frac{2}{N} \sum_{\vec{k}} (1 - \cos \vec{k}\vec{r}_i) \langle |\varphi_{\vec{k}}|^2 \rangle$$

$$= \frac{2}{N} \sum_{\vec{k}} (1 - \cos \vec{k}\vec{r}_i) \frac{kT}{2E} = \frac{kT}{Ja^2} \left(\frac{a}{2\pi}\right)^d \int d^d\vec{k} \frac{1 - \cos \vec{k}\vec{r}_i}{\vec{k}^2}.$$

1D-CASE:

$$\langle (\phi_i - \phi_0)^2 \rangle = \frac{kT}{\pi Ja} \int_0^\infty dk \frac{1 - \cos kr}{k^2} = r \frac{kT}{\pi Ja} \underbrace{\int_0^\infty dx \frac{1 - \cos x}{x^2}}_{=\gamma}$$

($x := kr$), so with a constant γ it is $G(r) = e^{-\gamma r/2} \to 0$ for $r \to \infty$ and the correlation length is $\xi = 2/\gamma \sim |T|^{-1}$.

3D-CASE:

$$\langle (\phi_i - \phi_0)^2 \rangle = \frac{akT}{(2\pi)^3 J} \int dk \, d\varphi \, d\theta \, k^2 \sin\theta \frac{1 - \cos(kr\cos\theta)}{k^2}$$

$$= \frac{akT}{(2\pi)^2 J} \frac{1}{r} \int_0^\infty dx \int_{-1}^1 d(\cos\theta) (1 - \cos(x\cos\theta))$$

($x := kr$). Obviously, this diverges. However, for the energy to be $E = Ja^2 \vec{k}^2$, the approximation $\vec{k} \ll 2\pi/a$ was necessary. Therefore, it is reasonable to impose a cut-off $x \ll kr \ll 2\pi r/a$:

$$\langle (\phi_i - \phi_0)^2 \rangle$$

$$= \frac{akT}{(2\pi)^2 J} \frac{1}{r} \int_0^{2\pi r/a} dx \int_{-1}^1 d(\cos\theta) (1 - \cos(x\cos\theta))$$

$$= \frac{kT}{\pi J} \left(1 - \frac{a}{2\pi r} \int_0^{2\pi r/a} dx \frac{1}{x}\sin x\right) \xrightarrow{r\to\infty} \frac{kT}{\pi J} = \text{const.}$$

Therefore, even for finite temperature there is a long range correlation: $G(r) \xrightarrow{r\to\infty} e^{-kT/2\pi J}$.

2D-CASE:

J_m is the Bessel-function. And again, one has to impose the cut-off (also for the lower boundary!) as for the 3D-case:

$$\langle (\phi_i - \phi_0)^2 \rangle = \frac{kT}{(2\pi)^2 J} \int dk \, d\theta \, k \frac{1 - \cos(kr\cos\theta)}{k^2}$$

$$= \frac{kT}{(2\pi)^2 J} \int dk \, d\theta \frac{1 - \sum_m J_m(kr) e^{im\theta}}{k}$$

$$= \frac{kT}{2\pi J} \int_b^{2\pi/a} dk \frac{1 - J_0(kr)}{k} = \frac{kT}{2\pi J} [\ln kr - Q(r)]_b^{2\pi/a}$$

$$= \frac{kT}{2\pi J} \left(\ln\frac{r}{a} + \tilde{Q}(r)\right) \xrightarrow{r\to\infty} \frac{kT}{2\pi J} \left(\ln\frac{r}{a} + \text{const.}\right)$$

(where $Q(r), \tilde{Q}(r)$ are some functions). Therefore, it is

$$G(r) \sim e^{-kT\ln(r/a)/4\pi J} \sim r^{-kT/4\pi J} \xrightarrow{r\to\infty} 0.$$

However, it is $G(r) \sim r^{-kT/4\pi J} e^{-r/\xi}$, it $\xi \to \infty$. Hence, although there is now correlation for $r \to \infty$, the correlation length is ∞!

8.3 Topological Excitation for a 2D System

TOPOLOGICAL CHARGES:

Writing $\phi(\vec{r}_i) := \phi_i$ gives a field $\phi(\vec{r})$ for for small $\vec{r}_i - \vec{r}_j$ it is

$$H \approx \frac{1}{2}J \sum_{\langle ij \rangle} \left(\phi(\vec{r}_i) - \phi(\vec{r}_j)\right)^2 \approx \frac{1}{2}J \sum_{\langle ij \rangle} |\nabla\phi|^2 \underbrace{(\vec{r}_i - \vec{r}_j)^2}_{\approx d^2 r}$$

$$\approx \frac{1}{2}J \int d^2r |\nabla\phi|^2.$$

If neighbouring spins vary only slightly from each other, the integration over closed loops gives

$$\oint d\vec{r} \, \nabla\phi = 2\pi\Phi,$$

where $\Phi \in \mathbb{Z}$ is the *topological charge*. This is because the spins might be changing direction ("turning") when on is moving along the loop, however in the last spin equals the first spin, so they have to turn an integer number of times. This charge is invariant under a small change of the spin states $\phi \to \phi + \delta\phi$:

$$\oint d\vec{r} \, \nabla\phi + \oint d\vec{r} \, \nabla\delta\phi = 2\pi\Phi,$$

since $\delta\phi \ll 1$ and the integral is integer (times 2π) it must be zero. $\phi = \psi + \varphi$ can always be separated into a curl-less part ψ and source-less part φ. The former describes spin waves and the latter vortices. With $\vec{V} := \nabla\varphi$ it is

$$\oint d\vec{r} \, \nabla\psi = \int d^2r \, \nabla \times \psi = 0, \quad \oint d\vec{r} \, \vec{V} = 2\pi\Phi = 2\pi \int d^2r \, \rho,$$

where ρ is the density of the topological charge Φ ($\rho := \Phi/s$ with area s). Using this notations, the Hamiltonian becomes

$$H \approx \frac{1}{2}J \int d^2r |\nabla\phi|^2$$

$$= \frac{1}{2}J \int d^2r \left(|\nabla\psi|^2 + |\vec{V}|^2\right) + \frac{1}{2}J \int d^2r |\nabla\psi||\nabla\varphi|,$$

where the last term is zero as can be shown by integration by parts. Since in 2D ony V_x and V_y exists, the Stokes theorem gives

$$\oint d\vec{r} \, \vec{V} = \int d^2r \, (\nabla \times \vec{V})\vec{e}_z = 2\pi \int d^2r \, \rho$$

$$\implies \quad (\nabla \times \vec{V})\vec{e}_z = \nabla(-\vec{e}_z \times \vec{V}) = 2\pi\rho,$$

which is similar to Gauss' law $\nabla\vec{E}_{\text{Gauss}} = \epsilon_0^{-1}\rho$. for an electric field $\vec{E}$. Thus one can define an "topological" electrostatic field

$$\vec{E} := -\vec{e}_z \times \vec{V} = (V_y, -V_x) \quad \implies \quad \nabla\vec{E} = 2\pi\rho.$$

The electrostatic energy is $\epsilon_0/2 \int d^3r \, \vec{E}_{\text{Gauss}}^2$ and hence

$$H_\varphi = \frac{J}{2} \int d^2r \, \vec{E}^2.$$

For a point charge $\rho = \Phi\delta(\vec{r})$, it is (in 2D-space!)

$$\vec{E} = \frac{\vec{r}}{r^2}\Phi = -\nabla U, \quad U = -\Phi \int_a^r dr' \frac{1}{r'} = -\Phi \ln\frac{r}{a} + \text{const.},$$

where the integration starts from the lattice constant a, since this is the smallest unit of space. The excitation energy of a single charge is (with system size L)

$$E(\Phi) = \frac{J}{2} \int d^2r \, \vec{E}^2 = \frac{J}{2}\Phi^2 \int d^2r \frac{1}{|\vec{r}|} = \pi J\Phi^2 \int_a^L dr' \frac{1}{r'}$$

$$= \pi J\Phi^2 \ln L/a.$$

For a pair of charges Φ_1 and Φ_2 at $\vec{r}_1$ and $\vec{r}_2$ the energy is

$$E_{12} = -2\pi J\Phi_1\Phi_2 \ln r_{12}/a + J\Phi_1\Phi_2 \cdot \text{const.}$$

CRITICAL TEMPERATURE:

The entropy S and free energy G per vortex is

$$S = k \ln L^2/a^2 = 2k \ln L/a, \quad G = (\pi J - 2kT) \ln L/a.$$

Hence, the critical temperature is

$$T_c = \frac{\pi J}{2k}$$

and for $T > T_c$ there are many topological charges. However, also for $T < T_c$ there might be *pairs* of positive and negative charges ("dipols"). The energy for a $+1, -1$ dipol is

$$E_d = 2\pi J \ln r/a + \pi^2 J.$$

Now the distance between the two pols of the dipol is

$$\langle r_{12}^2 \rangle = \frac{\int d^2r \, r^2 \, e^{-\beta E_p}}{\int d^2r \, e^{-\beta E_p}} = \frac{\int_a^L dr \, r^{3-4T_c/T}}{\int_a^L dr \, r^{1-4T_c/T}}$$

$$= a^2 \frac{2 - 4T_c/T}{4 - 4T_c/T} \frac{(L/a)^{4-4T_c/T} - 1}{(L/a)^{2-4T_c/T} - 1} = \begin{cases} a^2 \dfrac{2T_c - T}{2T_c - 2T} & \text{for } T < T_c \\ \infty & \text{for } T > T_c \end{cases}$$