Advanced Statistical Physics

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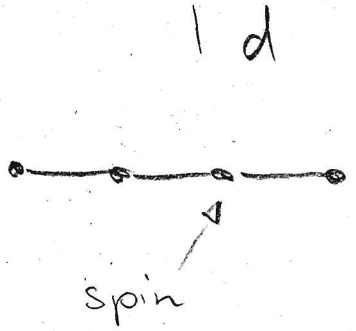
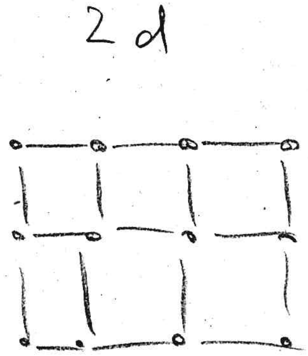
The Ising model

- model for ferromagnetism that emerges e.g. in Fe and Ni
- finite fraction of spins becomes spontaneously polarised in the same direction
- this gives rise to a macroscopic magnetic field
- however, this happens only when the temperature is sufficiently low, i.e. below the Curie temperature
- the Ising model allows to model and understand this phase transition behaviour
- it is one of very few statistical mechanics models with non-trivial behaviour that can be solved exactly

- the Ising model consists of N spins are pinned to the lattice sites of an d-dimensional periodic lattice ($d = 1, 2, 3$)





- the spin variable of a lattice site is denoted by s_i ($i = 1, .., N$)
- each variable s_i can assume two values

$$s_i = \begin{cases} +1 & \text{„spin up"} \\ -1 & \text{„spin down"} \end{cases}$$

- a given set of numbers $\{s_i\}$ denotes configuration (or microstate) of the whole system

- the energy of the system in the configuration $\{s_i\}$ is given by

$$E\{s_i\} = -\sum_{\langle ij\rangle} \varepsilon_{ij}\, s_i s_j - H\sum_{i=1}^{N} s_i$$

sum over nearest neighbours

interaction energy between i-th and j-th spin

field strength of an externally applied magnetic field

1d Ising model

- we assume spatially uniform interactions, i.e. $\varepsilon_{ij} = \varepsilon$
- the energy of a configuration is then

$$E = -\varepsilon \sum_{i=1}^{N} s_i s_{i+1} - H \sum_{i=1}^{N} s_i$$

- we assume periodic boundary conditions, such that $s_{N+1} = s_1$

- the canonical partition function is given by

$$Z = \mathrm{Tr}\, e^{-\beta E} = \sum_{s_1=\pm 1} \cdots \sum_{s_N=\pm 1} e^{\beta \varepsilon \sum_{i=1}^{N} s_i s_{i+1} + \beta H \sum_{i=1}^{N} s_i}$$

- we abbreviate: $h = \beta H$ and $K = \beta \varepsilon$
- this can be brought into a more convenient form by factorising the exponential

$$Z = \sum_{s_1} \cdots \sum_{s_N} \underbrace{\left[e^{\frac{h}{2}(s_1+s_2)+Ks_1s_2}\right]}_{T_{s_1s_2}} \times \underbrace{\left[e^{\frac{h}{2}(s_2+s_3)+Ks_2s_3}\right]}_{T_{s_2s_3}} \times \cdots \times \underbrace{\left[e^{\frac{h}{2}(s_N+s_1)+Ks_Ns_1}\right]}_{T_{s_Ns_1}}$$

- we can think of each term as being the elements of a matrix T, with

$$T_{s_1s_2} = e^{\frac{h}{2}(s_1+s_2)+Ks_1s_2}$$

$\hookrightarrow$ $$T = \begin{pmatrix} T_{11} & T_{1-1} \\ T_{-11} & T_{-1-1} \end{pmatrix} = \begin{pmatrix} e^{h+k} & e^{-k} \\ e^{-k} & e^{-h+k} \end{pmatrix}$$

- the partition function then becomes

$$Z = \sum_{s_1} \cdots \sum_{s_N} T_{s_1s_2} T_{s_2s_3} \cdots T_{s_Ns_1}$$

- T is called the transfer matrix

- using the fact that matrix multiplication is defined as $A = B \cdot C \leftrightarrow A_{ij} = \sum_k B_{ik} C_{kj}$, and that the trace of a matrix is defined as $\mathrm{Tr}(A) = \sum_i A_{ii}$, we can write

$$Z = \sum_{S_1} (T \cdot T \ldots T)_{S_1 S_1} = \sum_{S_1} (T^N)_{S_1 S_1} = \mathrm{Tr}\, T^N$$

↳ the partition function is given by the trace of the N-th power of the transfer matrix T

- we can calculate Z explicitly by diagonalising T with a similarity transformation:

$$T = S T' S^{-1} = S \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} S^{-1},$$

with $\lambda_{1/2}$ being the eigenvalues of T

- note, that $\mathrm{Tr}(T^N) = \mathrm{Tr}(T T \ldots T)$

$$= \mathrm{Tr}(S T' \underbrace{S^{-1} S}_{1} T' S^{-1} \ldots S T' S^{-1})$$

$$= \mathrm{Tr}(S T' T' \ldots S^{-1}) = \mathrm{Tr}(\underbrace{S^{-1} S}_{1} T' \ldots T')$$

$$= \mathrm{Tr}\, T'^N$$

- we can thus write

$$Z = \mathrm{Tr}\, T^N = \mathrm{Tr} \begin{pmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{pmatrix} = \lambda_1^N + \lambda_2^N$$

- assuming that $\lambda_1 > \lambda_2$, we have

$$Z = \lambda_1^N \left(1 + \left[\frac{\lambda_2}{\lambda_1} \right]^N \right) \xrightarrow{N \gg 1} \lambda_1^N$$

↳ in the thermodynamic limit only the largest eigenvalue of the transfer matrix T is important

- we can now compute the free energy:

$$F = -\frac{1}{\beta} \log Z = -N \frac{1}{\beta} \log \lambda_1$$

- in order to obtain an explicit expression we need to find the eigenvalues of the transfer matrix:

$$0 = \begin{vmatrix} e^{h+k} - \lambda & e^{-k} \\ e^{-k} & e^{-h+k} - \lambda \end{vmatrix} = (e^{h+k} - \lambda)(e^{-h+k} - \lambda) - e^{-2k}$$

$$= \lambda^2 - 2\lambda e^k \cosh(h) + 4 \cosh(k) \sinh(k)$$

- the two solutions of the characteristic polynomial are

$$\lambda_1 = e^{K}\left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4K}}\right)$$

$$\lambda_2 = e^{K}\left(\cosh(h) - \sqrt{\sinh^2(h) + e^{-4K}}\right)$$

- the free energy of the 1d Ising model thus becomes (with $\beta = 1/k_BT$)

$$\frac{F}{N} = -\frac{1}{\cancel{\beta}}\beta\varepsilon - \frac{1}{\beta}\log\left(\cosh(\beta H) + \sqrt{\sinh^2(\beta H) + e^{-4\beta\varepsilon}}\right)$$

<u>Thermodynamic properties of the 1d Ising model</u>

- in the absence of an external magnetic field ($H=0$) we have

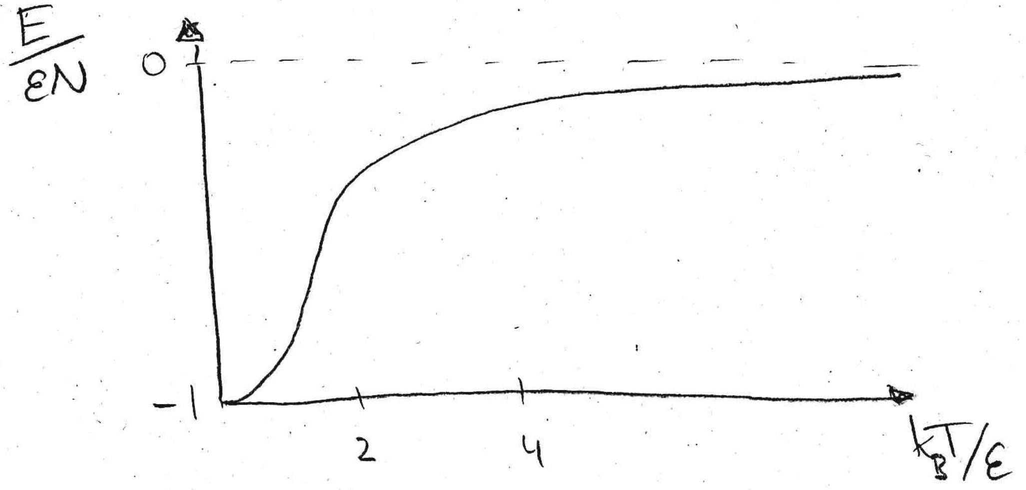
$$\frac{F}{N} = \underbrace{-\varepsilon}_{\substack{\text{energetic part;} \\ \text{dominates @ } T\to 0 \\ (\beta\to\infty)}} \underbrace{- \frac{1}{\beta}\log\left(1 + e^{-2\beta\varepsilon}\right)}_{\substack{\text{entropic part;} \\ \text{dominates @ } T\to\infty \\ (\beta\to 0)}}$$

$$F = E - TS$$

- internal energy:

$$E = -\frac{\partial}{\partial\beta}\log Z = -\frac{\partial}{\partial\beta}\log\left(e^{k}+e^{-k}\right)^{N} = -\frac{\partial}{\partial\beta}\log\left[2\cosh(\beta\varepsilon)\right]^{N}$$

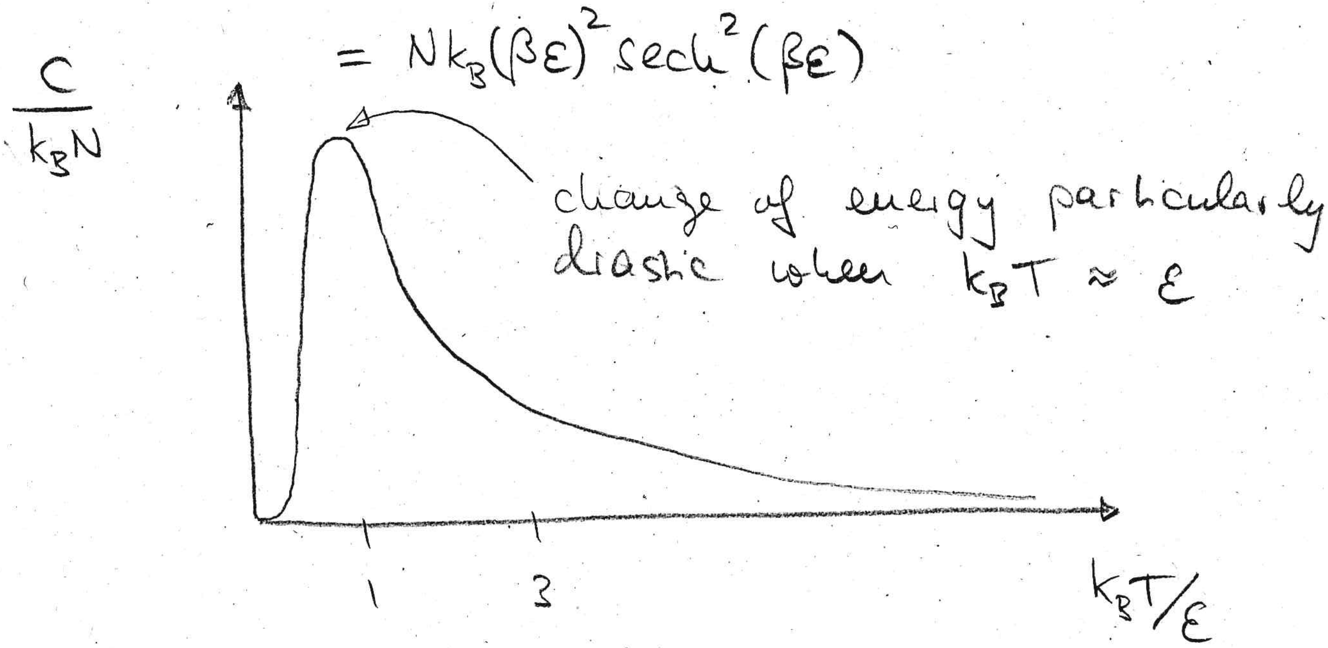
$$= -N\frac{\partial}{\partial\beta}\log 2\cosh(\beta\varepsilon) = -N\varepsilon\tanh(\beta\varepsilon)$$



- specific heat:

$$C = \frac{dE}{dT} = -\frac{1}{k_BT^2}\frac{dE}{d\beta} = \frac{N\varepsilon^2}{k_BT^2}\operatorname{sech}^2\left(\varepsilon/k_BT\right)$$

$$= Nk_B(\beta\varepsilon)^2\operatorname{sech}^2(\beta\varepsilon)$$

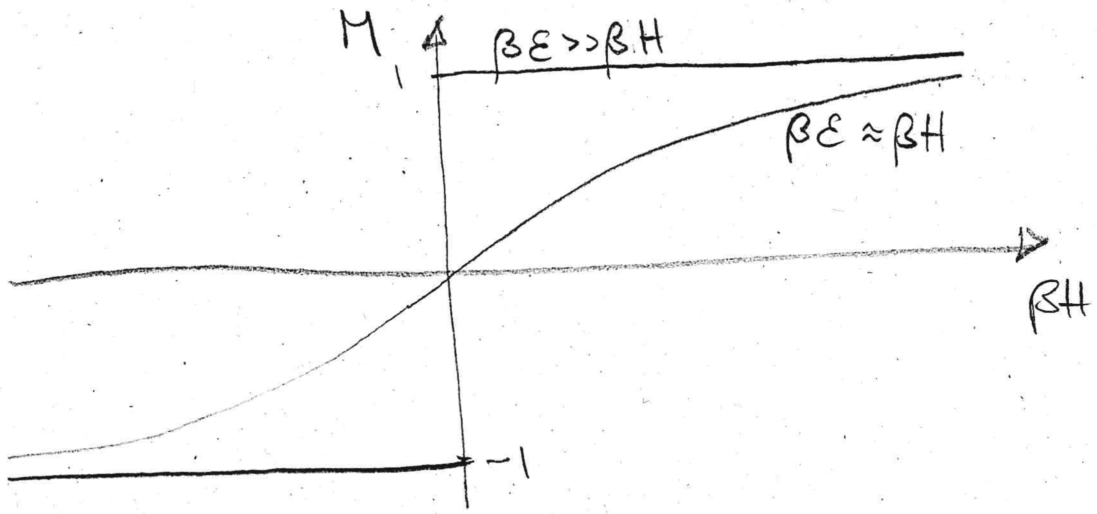


- peak is the so-called Schottky anomaly
- characteristic for systems with discrete energy levels

- magnetisation (requires consideration of finite H): (9)

$$M = -\frac{1}{N}\frac{\partial F}{\partial H} = -\frac{\beta}{N}\frac{\partial F}{\partial h} = \frac{\partial}{\partial h}\log\left[\cosh(h) + \sqrt{\sinh^2(h)+e^{-4K}}\right]$$

$$= \frac{\sinh(h)}{\sqrt{\sinh^2(h)+e^{-4K}}} = \frac{\sinh(\beta H)}{\sqrt{\sinh^2(\beta H)+e^{-4\beta\varepsilon}}}$$



- when $\beta\varepsilon \gg \beta H$ the magnetisation jumps at $\beta H = 0$, i.e. it becomes a non-analytic function of the magnetic field
- to understand this a bit better, lets take a look at the largest eigenvalue of the transfer matrix in the limit where $\beta\varepsilon \gg 1$ and βH finite

(T goes to zero and H changes in a way that H/T remains finite)

- here we can write

$$\lambda_1 = e^{\beta\epsilon}\left[\cosh(\beta H) + \sqrt{\sinh^2(\beta H)}\,(1+\mathcal{O}(e^{-4\beta\epsilon}))\right]$$

and hence

$$\lambda_1 \approx e^{\beta\epsilon}\underbrace{\left[\cosh(\beta H) + |\sinh(\beta H)|\right]}_{e^{|\beta H|}} = e^{\beta\epsilon + \beta|H|}$$

- the free energy then becomes

$$F = -N(\epsilon + |H|),$$

and thus the magnetisation is

$$M = -\frac{1}{N}\frac{\partial F}{\partial H} = \begin{cases} 1, & H>0 \\ -1, & H<0 \end{cases}$$

- for any finite T the magnetisation at $H=0$ is zero

↳ for $T=0$ there is a spontaneous magnetisation, with the direction set by an infinitesimally small magnetic field:

$$\lim_{H\to 0^-} M = -1 \qquad \lim_{H\to 0^+} M = +1$$

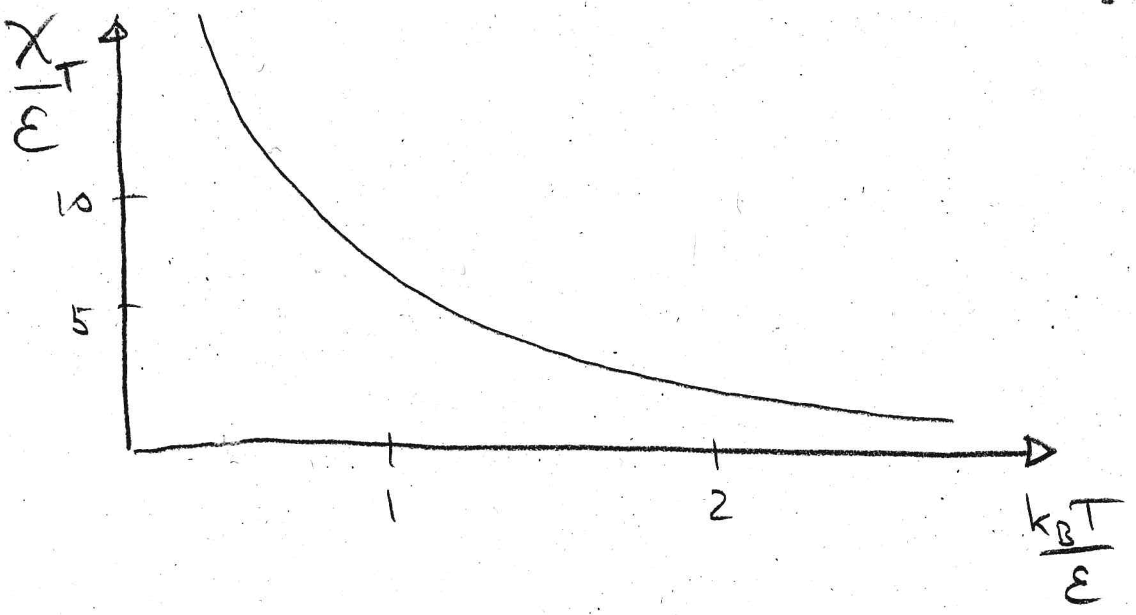
- isothermal susceptibility:
- describes how magnetisation changes in response to a magnetic field

$$\chi_T = \frac{\partial M}{\partial H} = \beta \frac{\partial}{\partial h} \frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4\beta\varepsilon}}}$$

- for small h we have $\sinh(h) \approx h$

and $\chi_T \approx \beta \frac{\partial}{\partial h} \frac{h}{e^{-2\beta\varepsilon}} = \beta e^{2\beta\varepsilon}$

$$= \frac{e^{2\frac{\varepsilon}{k_B T}}}{k_B T}$$



- for high temperatures one find Curie's law: $\chi_T \sim \frac{1}{k_B T}$

- Spatial correlations:

- the two-point correlation function is defined as

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

where $\langle A \rangle = \dfrac{\mathrm{Tr}\, A\, e^{-\beta E}}{\mathrm{Tr}\, e^{-\beta E}}$ denotes the expectation value of the quantity A

- the correlation function can be rewritten as $G_{ij} = \langle (S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle) \rangle$, which shows that it measures the correlation in the fluctuations of the spins at different sites (labelled by i and j)

- we use the transfer matrix method to calculate G_{ij}

- to this end we use

$$\langle S_i \rangle = \frac{1}{Z} \sum_{S_1} \dots \sum_{S_N} e^{-\beta E} S_i$$

$$= \frac{1}{Z} \sum_{S_1} \dots \sum_{S_N} T_{S_1 S_2} T_{S_2 S_3} \dots T_{S_{i-1} S_i} S_i T_{S_i S_{i+1}} \dots$$

- we focus on the string

$$B_{s_{i-1} s_{i+1}} = \sum_{s_i} T_{s_{i-1} s_i} \, s_i \, T_{s_i s_{i+1}}$$

$$= \left[T \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} T \right]_{s_{i-1} s_{i+1}}$$

- the matrix $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is a Pauli matrix which is typically denoted by σ_z.
- hence we can write

$$\langle s_i \rangle = \frac{1}{Z} \operatorname{Tr} (\sigma_z T^N) = \frac{\operatorname{Tr} \left[S^{-1} \sigma_z S (T')^N \right]}{\operatorname{Tr} \left[(T')^N \right]}$$

- this can be explicitly solved
- here we just use that we can generally write $S^{-1} \sigma_z S = \begin{pmatrix} \alpha_1 & \alpha_3 \\ \alpha_4 & \alpha_2 \end{pmatrix}$, and hence

$$\langle s_i \rangle = \frac{\alpha_1 \lambda_1^N + \alpha_2 \lambda_2^N}{\lambda_1^N + \lambda_2^N} \xrightarrow{N \gg 1} \alpha_1$$

- Similarly, the two-point correlations can be written as

$$\langle s_i s_{i+j} \rangle = \frac{1}{Z} \operatorname{Tr} \left[(S^{-1} \sigma_z S) (T')^j (S^{-1} \sigma_z S) (T')^{N-j} \right]$$

- in the limit $N \gg 1$ this yields

$$\langle S_i S_{i+j} \rangle = \alpha_1^2 + \alpha_3 \alpha_4 \left(\frac{\lambda_2}{\lambda_1}\right)^j$$

- therefore, the correlation function becomes

$$G_{i,i+j} = \langle S_i S_{i+j} \rangle - \langle S_i \rangle \langle S_{i+j} \rangle = \alpha_3 \alpha_4 \left(\frac{\lambda_2}{\lambda_1}\right)^j$$

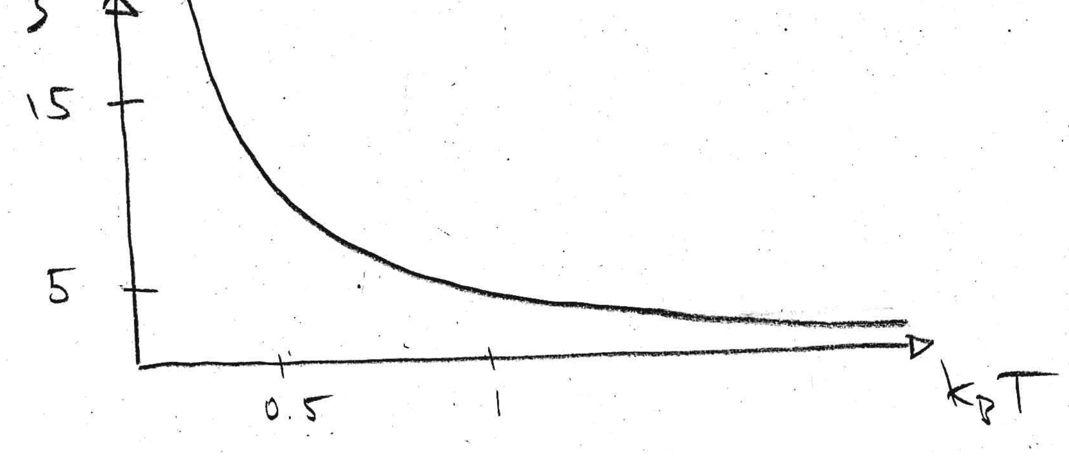
$$= \alpha_3 \alpha_4 \, e^{-j/\xi}$$

with the correlation length

$$\xi = \frac{1}{\log \frac{\lambda_1}{\lambda_2}}$$

- in the absence of a magnetic field, we have $\lambda_1 = 2\cosh \beta\varepsilon$, $\lambda_2 = 2\sinh \beta\varepsilon$.

- hence, $\xi = \dfrac{1}{\log(\coth(\beta\varepsilon))} = \dfrac{1}{\log\left(\coth\left(\frac{\varepsilon}{k_B T}\right)\right)}$



remarks:

- the correlation length ξ cannot diverge unless $\lambda_1 = \lambda_2$, i.e. there has to be a degeneracy of the largest eigenvalue for this to happen $\longrightarrow$ this signals a phase transition

- in the 1d Ising model we have for $H \neq 0$, $\lambda_1 > \lambda_2$; so there cannot be a phase transition when $H \neq 0$

- for $H = 0$, $\lambda_1 = \lambda_2$ when $\beta\varepsilon \to \infty$, i.e. $T \to 0$

  ↳ the 1d Ising model does not show a phase transition at finite temperature!

- the absence of a phase transition in the 1d Ising model (at finite T) and generally in 1d models with short range interactions can also be established via <u>Perron's theorem</u>

For an $N \times N$ matrix ($N < \infty$) T with $T_{ij} > 0 \; \forall i,j$ the eigenvalue of largest magnitude is:

(a) real and positive

(b) non-degenerate

(c) an analytic function of T_{ij}

↳ 1d models with short range interactions have (at finite temperature) a transfer matrix that satisfies the above-mentioned conditions

↳ no phase transition in 1d

- for the Ising model one can make a simple argument based on the free energy, which shows that a fully magnetised state is unstable under arbitrarily small thermal fluctuations

- the state $\uparrow\uparrow\uparrow\uparrow\uparrow$ has energy $-N\varepsilon$ and zero entropy

↳ free energy: $F_{\uparrow\uparrow\uparrow\uparrow} = -N\varepsilon$

- the (set of) states with one domain wall, $\uparrow\uparrow\uparrow\downarrow\downarrow$ have energy $-N\varepsilon + 2\varepsilon$ and an entropy of $S = k_B \log N$, since the domain wall can be on N different positions.

$$\hookrightarrow F_{\uparrow\uparrow\downarrow\downarrow} = -N\varepsilon + 2\varepsilon - k_B T S$$

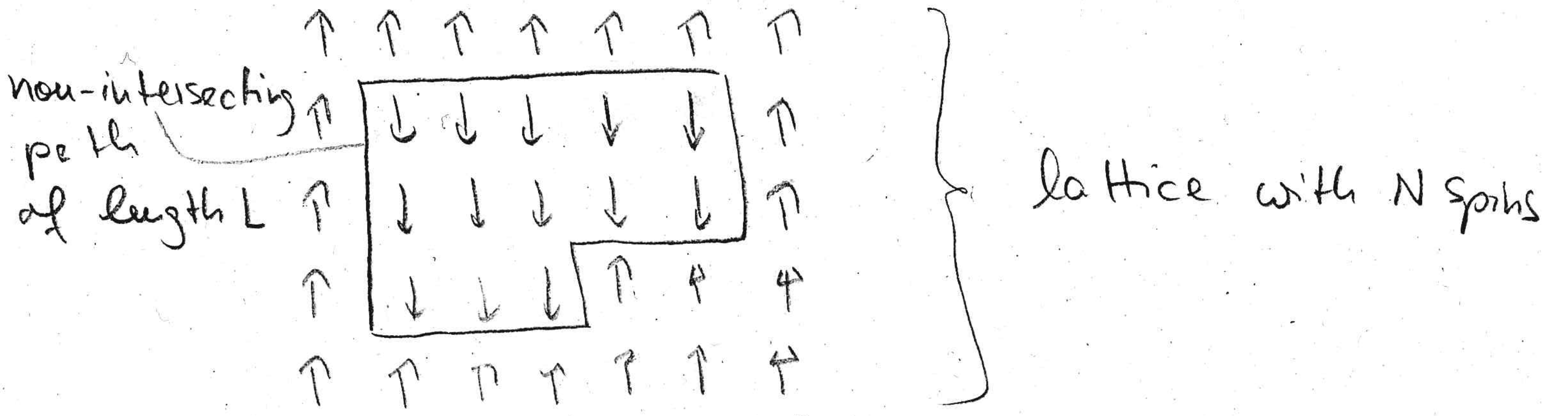
↳ $\Delta F = F_{\uparrow\uparrow\downarrow\downarrow} - F_{\uparrow\uparrow\uparrow\uparrow} = 2\varepsilon - k_B T \log N$

↳ for large N and finite T it is always favourable to create domain walls

→ fully magnetised state is unstable

2d Ising model

- to extend the previous argument to two dimensions we consider a domain of down-spins embedded in a background of up-spins



- the energy cost to create the domain boundary from a fully magnetised state is $\Delta E(L) = 2\varepsilon L$, with L being the length of the boundary (= number of $\downarrow\uparrow$ or $\uparrow\downarrow$ links)
- in order to calculate the entropy increase one needs to calculate the number of closed domain boundaries of length L $(= \Gamma(L))$

- we will give an upper bound for this quantity
- imagine we start drawing a boundary at a random link : 
- in the next step we continue the boundary in a random direction without going back, i.e. we have 3 possible choices 

- for a path of length L we thus have 3^{L-1} choices
- moreover, we can start from any of the N lattice sites
- therefore, $\Gamma < N\,3^{L-1}$ since the number of paths of length L is larger than the number of closed non-intersecting paths of length L

$$\hookrightarrow \Delta S < k_B \log(N\,3^{L-1}) = k_B \log N + k_B (L-1) \log 3$$

↳ free energy difference:

$$\Delta F \approx 2\varepsilon L - k_B T (L-1)\log 3 - k_B T \log N$$

$$= L\left[2\varepsilon - k_B T \log 3\right] + \underbrace{\frac{k_B T \log 3}{L} - \frac{k_B T \log N}{L}}_{\substack{\text{negligible when} \\ L,N \gg 1 \ \& \ L \sim N}}$$

- hence, there is a finite critical temperature $T_c \sim \frac{\varepsilon}{k_B}$ below which the free energy change becomes positive and the fully magnetised state becomes stable against the formation of domains

Mean field theory

- this is not an exact treatment, but it gives an idea about the behaviour of the Ising model in higher dimensions

- we start with the non-interacting Ising model

$$E_0\{S_i\} = -H \sum_{i=1}^{N} S_i$$

$$\hookrightarrow \quad Z_0 = \prod_{i=1}^{N} \left(e^{\beta H} + e^{-\beta H} \right) = 2^N \cosh^N\left(\frac{H}{k_B T}\right)$$

- the magnetisation evaluates to

$$M = -\frac{1}{N}\frac{\partial F}{\partial H} = \tanh\left(\frac{H}{k_B T}\right) = \frac{1}{N}\sum_i \langle S_i \rangle$$

- the idea behind mean field is to write the interactions in a way which pretends that each spin experiences a magnetic field which is given by the mean magnetisation of its neighbours

$$E_{int}\{S_i\} = -\varepsilon \sum_{\langle ij \rangle} S_i S_j \approx -\varepsilon \sum_{\langle ij \rangle} S_i \langle S_j \rangle$$

$$\approx -\varepsilon \sum_{\langle ij \rangle} S_i \underbrace{M}_{\text{magnetisation, assuming that system is homogeneous}} = -\varepsilon \underbrace{2d}_{\text{coordination number: } 2\times \text{ dimension for hypercubic lattice}} M \sum_i S_i$$

- the mean field energy is thus

$$E_{MF}\{S_i\} = E_0\{S_i\} - 2\varepsilon d M \sum_i S_i$$

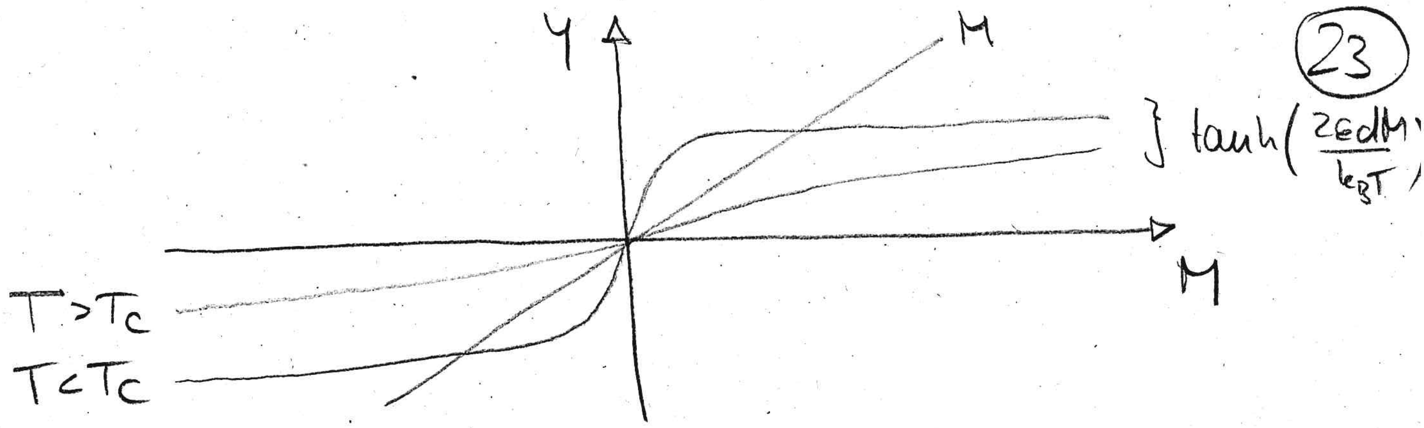
$$= -(H + 2\varepsilon d M) \sum_i S_i$$

- this is a non-interacting problem, and one can readily calculate the partition function and magnetisation:

$$M = \tanh\left(\frac{H + 2\varepsilon d M}{k_B T}\right)$$

- setting $H = 0$, we can now investigate under which conditions this equation has a solution which is not $M = 0$

↳ this will signal the emergence of a spontaneous magnetisation



- the curves $y = M$ & $y = \tanh\left(\frac{2\varepsilon d M}{k_B T}\right)$ only have a crossing point other than $M = 0$, when

$$T < T_c = \frac{2d\varepsilon}{k_B} \quad \Big\} \text{ mean field critical temperature}$$

Behaviour near the critical temperature

- it is instructive to investigate the behaviour of the magnetisation near the critical temperature
- in fact, understanding this „critical behaviour" is one important way to characterise and classify phase transitions

- for this analysis we write

$$M = \tanh\left(\frac{H}{k_BT} + M\frac{T_c}{T}\right) = \frac{\tanh\left(\frac{H}{k_BT}\right) + \tanh\left(M\frac{T_c}{T}\right)}{1 + \tanh\left(\frac{H}{k_BT}\right)\tanh\left(M\frac{T_c}{T}\right)}$$

$$\hookrightarrow \tanh\frac{H}{k_BT} = \frac{M - \tanh\left(M\frac{T_c}{T}\right)}{1 - M\tanh\left(M\frac{T_c}{T}\right)}$$

- near the critical temperature the magnetisation is small, $M \ll 1$
- moreover, we assume that the magnetic field is small, $H \ll 1$
- we can thus Taylor expand the functions

$$\hookrightarrow \frac{H}{k_BT} \approx M\left(1 - \frac{T_c}{T}\right) + M^3\left(\frac{T_c}{T} - \left(\frac{T_c}{T}\right)^2 + \frac{1}{3}\left(\frac{T_c}{T}\right)^3\right) + \mathcal{O}(M^5)$$

- at $H = 0$ we thus find:

$$M^2 \approx -\frac{1 - \frac{T_c}{T}}{\frac{T_c}{T} - \left(\frac{T_c}{T}\right)^2 + \frac{1}{3}\left(\frac{T_c}{T}\right)^3} \approx 3\left(1 - \frac{T}{T_c}\right)$$

- hence, near the critical temperature, the magnetisation follows a power law

$$M \sim \left(1 - \frac{T}{T_c}\right)^\beta \quad \text{with } \beta = 1/2$$

- β is a so-called critical exponent
- the magnetisation as a function of H follows a similar behaviour
- setting $T = T_c$ and allowing $H \neq 0$ leads to

$$\frac{H}{k_B T} \sim M^3 \longrightarrow M \sim H^{1/\delta}$$

with $\delta = 3$

- δ is a further critical exponent
- the isothermal susceptibility χ_T diverges near T_c following a power law

$$\hookrightarrow \underbrace{\frac{\partial}{\partial H} \frac{H}{k_B T}}_{= \frac{1}{k_B T}} \approx \underbrace{\frac{\partial}{\partial H} M}_{\chi_T} \left(1 - \frac{T_c}{T}\right) + 3M^2 \underbrace{\frac{\partial M}{\partial H}}_{\chi_T} \left(\frac{T_c}{T} - \left(\frac{T_c}{T}\right)^2 + \frac{1}{3}\left(\frac{T_c}{T}\right)^3\right)$$

$$\hookrightarrow \chi_T = \frac{1}{k_B} \frac{1}{(T - T_c)^\gamma}$$ with $\gamma = 1$ for $T > T_c$ and $M = 0$

- for $T < T_c$ one has $M = \sqrt{3} \left(\frac{T_c - T}{T_c}\right)^{1/2}$
- substituting this into the above equation and solving for χ_T leads to

$$\chi_T = \frac{1}{k_B} \frac{1}{(T_c - T)^{\gamma'}}$$ with $\gamma' = 1$

- the susceptibility χ_T diverges here with the same power law no matter whether one approaches the critical point from above or below

Susceptibility and spatial correlations

- the divergence of χ_T has an interesting connection to the correlation length, which we discussed already in the context of the 1d Ising model
- to see this we calculate χ_T using the partition function Z

$$\chi_T = \frac{\partial M}{\partial H} = \frac{1}{N\beta}\frac{\partial^2 \log Z}{\partial H^2} = \frac{k_B T}{N}\left[\frac{1}{Z}\frac{\partial^2 Z}{\partial H^2} - \frac{1}{Z^2}\left(\frac{\partial Z}{\partial H}\right)^2\right]$$

- now $\frac{k_B T}{Z}\frac{\partial Z}{\partial H} = \sum_i \langle S_i \rangle$

and $\frac{(k_B T)^2}{Z}\frac{\partial^2 Z}{\partial H^2} = \sum_{ij} \langle S_i S_j \rangle$

- these relations permit to connect χ_T with the correlation function

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

$$\chi_T = \frac{1}{Nk_BT}\left[\sum_{ij}\langle S_i S_j\rangle - \underbrace{\left(\sum_i \langle S_i\rangle\right)^2}_{=\sum_{ij}\langle S_i\rangle\langle S_j\rangle}\right]$$

$$= \frac{1}{Nk_BT}\sum_{ij} G_{ij}$$

dimension

assuming translation invariance

$$= \frac{1}{k_BT}\sum_j G_{ij} \approx \frac{1}{k_BTa^d}\int d^d r\, G(r)$$

characteristic microscopic length scale (lattice spacing)

- we saw for the 1d Ising model that $G(r) \sim e^{-r/\xi}$ with ξ being the correlation length

$\longrightarrow$ χ_T is always finite unless ξ diverges and hence the integral as well (for the 1d Ising model this happens at $T=0$)

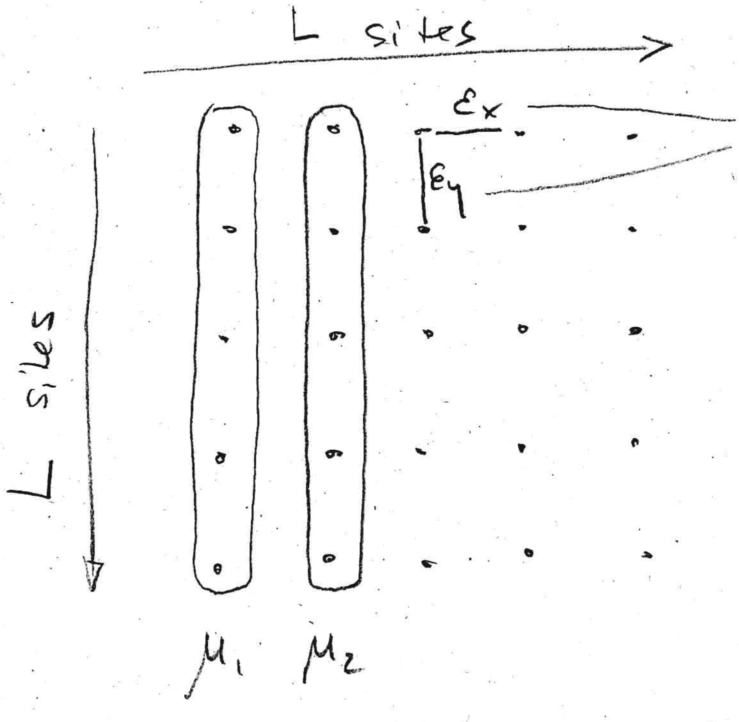
$\hookrightarrow$ generally a diverging χ_T signals a diverging correlation length

Solution to the 2d Ising model

- 2d Ising model is exactly solvable as shown by Onsager
- we will sketch the main steps, but won't follow this solution to the very end
- instead we will establish a connection between the 2d Ising model and the quantum 1d Ising model, which will allow us to establish and analyse the presence of a phase transition

Setting:

2d lattice with periodic boundary conditions



consider the possibility of anisotropic couplings

- the state of a column is denoted by the L-dimensional vector

$$\mu = \{ s_1, \dots, s_L \}$$

- denoting the state of the adjacent column as $\mu' = \{ s_1', \dots, s_L' \}$ and introducing the energies

$$E(\mu, \mu') = -\varepsilon_x \sum_{k=1}^{L} s_k s_k'$$

and $E(\mu) = -\varepsilon_y \sum_{k=1}^{L} s_k s_{k+1}$

the Ising energy function can be written as

$$E\{\mu_1, \dots, \mu_L\} = \sum_{\alpha=1}^{L} \left(E(\mu_\alpha, \mu_{\alpha+1}) + E(\mu_\alpha) \right)$$

- the partition function then becomes

$$Z = \sum_{\mu_1} \dots \sum_{\mu_L} \exp\left\{ -\beta \sum_{\alpha=1}^{L} \left(E(\mu_\alpha, \mu_{\alpha+1}) + E(\mu_\alpha) \right) \right\}$$

- defining the matrix P with

$$\langle \mu | P | \mu' \rangle = e^{-\beta (E(\mu, \mu') + E(\mu))}$$

we can rewrite the partition function as

$$Z = \sum_{\mu_1 \cdots \mu_L} \langle \mu_1 | P | \mu_2 \rangle \langle \mu_2 | P | \mu_3 \rangle \cdots \langle \mu_L | P | \mu_1 \rangle$$

$$= \sum_{\mu_1} \langle \mu_1 | P^L | \mu_1 \rangle = \mathrm{Tr}\, P^L$$

$$= \sum_{k=1}^{2^L} (\lambda_k)^L$$ with λ_k being the eigenvalues of P

- in analogy to 1d case we expect that in the thermodynamic limit, $L \to \infty$, the largest eigenvalue will dominate, and hence

$$Z \sim \lambda_{max}^L$$

- let us now investigate the structure of P more closely
- the matrix elements of P are

$$\langle S_1, \ldots, S_L | P | S_1', \ldots, S_L' \rangle = \prod_{k=1}^{L} e^{\beta \varepsilon_y S_k S_{k+1}} e^{\beta \varepsilon_x S_k S_k'}$$

- we now define two matrices, V_1 and V_2, with elements

$$\langle S_1, \ldots, S_L | V_1 | S_1', \ldots, S_L' \rangle = \prod_{k=1}^{L} e^{\beta \varepsilon_x S_k S_k'}$$

$$\langle S_1, \ldots, S_L | V_2 | S_1', \ldots, S_L' \rangle = \delta_{S_1 S_1'} \cdots \delta_{S_L S_L'} \prod_{k=1}^{L} e^{\beta \varepsilon_y S_k S_{k+1}}$$

- this allows us to write $P = V_2 V_1$

- V_1 can actually be written as a direct product: $V_1 = v \otimes v \otimes \dots \otimes v$ where the matrix v has the element

$$\langle s | v | s' \rangle = e^{\beta \varepsilon_x s s'}$$

- this is in fact the transfer matrix of the 1d Ising model at zero magnetic field

$$\hookrightarrow \quad v = \begin{pmatrix} e^{\beta\varepsilon_x} & e^{-\beta\varepsilon_x} \\ e^{-\beta\varepsilon_x} & e^{\beta\varepsilon_x} \end{pmatrix} = e^{\beta\varepsilon_x}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + e^{-\beta\varepsilon_x}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= e^{\beta\varepsilon_x}\mathbb{1} + e^{-\beta\varepsilon_x}\sigma_x$$ ← Pauli matrix

- we can bring this into a more convenient form using the formula

$$e^{\theta\sigma_x} = \cosh\theta\,\mathbb{1} + \sinh\theta\,\sigma_x = \cosh\theta\,(1 + \tanh\theta\,\sigma_x)$$

$$\hookrightarrow \quad v = \underbrace{\frac{e^{\beta\varepsilon_x}}{\cosh\theta}}_{=\sqrt{2\sinh(2\beta\varepsilon_x)}} e^{\theta\sigma_x} \qquad \text{with } \tanh\theta = e^{-2\beta\varepsilon_x}$$

- one thus finds that

$$V_1 = \left[2\sinh(2\beta\varepsilon_x)\right]^{L/2} e^{\theta\sum_{k=1}^{L}\sigma_x^k} \qquad \text{where } \sigma_x^k = \mathbb{1}\otimes\dots\otimes\underset{\substack{\uparrow \\ k\text{-th position}}}{\sigma_x}\otimes\dots\otimes\mathbb{1}$$

- the matrix V_2 is a diagonal matrix which can be represented using the Pauli matrix $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- this is achieved by noticing that

$$e^{\beta\varepsilon_y S_1 S_2}\,\delta_{S_1 S_1'}\,\delta_{S_2 S_2'} = \langle S_1 S_2 | e^{\beta\varepsilon_y \sigma_z^1 \sigma_z^2} | S_1' S_2' \rangle$$

$$\hookrightarrow \quad V_2 = e^{\beta\varepsilon_y \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}}$$

- hence, the transfer matrix P of the 2d Ising model is

$$P = V_2 V_1 = \left[\sinh(2\beta\varepsilon_x)\right]^{L/2} e^{\beta\varepsilon_y \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}}\, e^{\theta \sum_{k=1}^{L} \sigma_x^k}$$

with $\tanh\theta = e^{-2\beta\varepsilon_x}$

- the largest eigenvalue of P can be found analytically, see book by Huang
- in the following we briefly discuss the solution for the isotropic case, $\varepsilon_x = \varepsilon_y$

- <u>free energy per spin:</u>

$$\beta \frac{F}{L^2} = -\log\left[2\cosh(2\beta\varepsilon)\right] - \frac{1}{2\pi}\int_0^{\pi} d\phi \, \log\left[\frac{1}{2}\left(1+\sqrt{1-k^2\sin^2\phi}\right)\right]$$

$$\text{with} \quad k = \frac{2}{\cosh(2\beta\varepsilon)\coth(2\beta\varepsilon)}$$

- <u>energy per spin:</u>

$$\frac{E}{N^2} = \frac{\partial}{\partial\beta}\left(\frac{\beta F}{L^2}\right) = -\varepsilon\coth(2\beta\varepsilon)\left[1+\frac{2}{\pi}\left(2\tanh^2(2\beta\varepsilon)-1\right)K_1(k)\right]$$

where $K_1(k) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1-k^2\sin^2\phi}}$ is the complete elliptic integral of the first kind

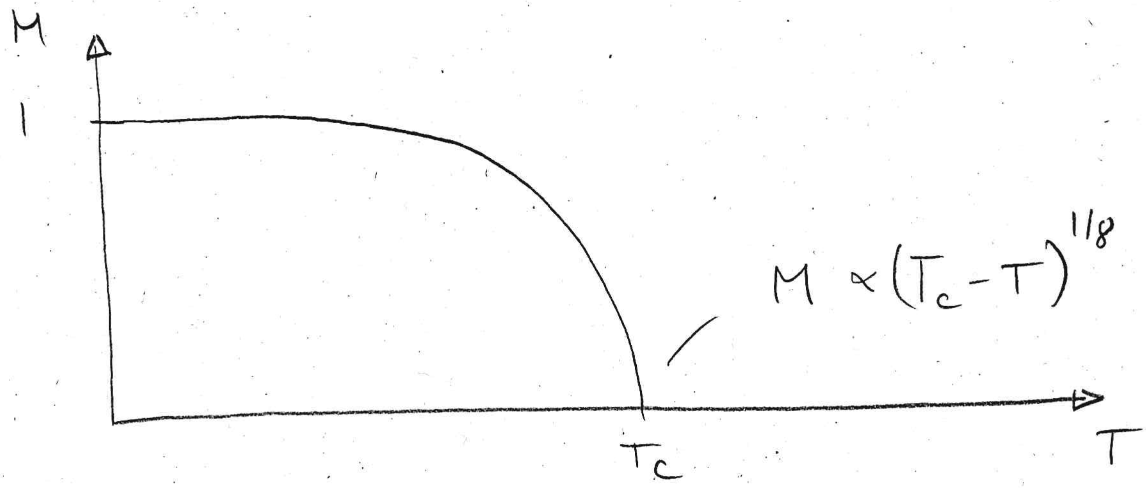
- $K_1(k)$ has a singularity at $k=1$, which determines the critical temperature

$$\hookrightarrow \quad 1 = \frac{2}{\cosh(2\beta_c\varepsilon)\coth(2\beta_c\varepsilon)}$$

$$\hookrightarrow \quad \frac{1}{\beta_c} = k_B T_c = \frac{2\varepsilon}{\log(1+\sqrt{2})} \approx 2.27 \cdot \varepsilon$$

- magnetisation:

$$M = \begin{cases} 0 & , \quad T > T_c \\ \{1 - [\sinh(2\beta\varepsilon)]^{-4}\}^{1/8} & , \quad T < T_c \end{cases}$$



- magnetisation emerges spontaneously below T_c (note, that there is a symmetry: $M \to -M$)
- near T_c the magnetisation behaves as $M \propto (T_c - T)^\beta$ with $\beta = 1/8$

  ↳ the critical exponent is different from the mean field prediction

- other critical exponents

	mean field	2d Ising	3d Ising
β	$1/2$	$1/8$	0.325
δ	3	15	4.82
γ	1	$7/4$	1.241

Connection to quantum 1d Ising model

- the partition function of the 2d Ising model is

$$Z \propto \mathrm{Tr}\left[e^{\beta\varepsilon_y \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}} \, e^{\operatorname{arctanh} e^{-2\beta\varepsilon_x} \sum_{k=1}^{L} \sigma_x^k} \right]^L$$

- in the following we consider the limit in which $\varepsilon_y \ll 1$ and $\varepsilon_x \gg 1$, i.e. weak coupling along a column and strong coupling between the rows

- we parameterise

$$\beta\varepsilon_y = \gamma\Delta\tau \quad \text{and} \quad \operatorname{arctanh} e^{-2\beta\varepsilon_x} \approx e^{-2\beta\varepsilon_x} = \Delta\tau$$

with $\Delta\tau \ll 1$

- this allows us to expand the two exponentials of the partition function: $e^x \approx 1 + x \ldots$

$$\hookrightarrow Z \sim \mathrm{Tr}\left[1 + \Delta\tau\gamma \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1} + \Delta\tau \sum_{k=1}^{L} \sigma_x^k + \ldots \right]^L$$

$$\approx \mathrm{Tr} \exp\left[-\underbrace{\Delta\tau L}_{\beta_{eff}} H \right]$$

- here $H = -\sum_{k=1}^{L} \sigma_x^k - \gamma \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}$

is the Hamiltonian of a 1d quantum Ising model in a transverse field of field strength 1

- the interaction strength between neighbouring spins is $\gamma = \beta \varepsilon_y e^{2\beta \varepsilon_x}$
- the effective temperature $(\beta_{eff})^{-1} = (\Delta\tau L)^{-1}$ tends to zero in the thermodynamic limit

↳ • phase transition in the 2d Ising model corresponds in the considered limit to quantum phase transition in the ground state of the quantum Hamiltonian H

- here the excitation gap of H closes, i.e. the ground state energy becomes degenerate with energy of excited states
- in turn this means that the largest eigenvalues of the transfer matrix become degenerate

- the Hamiltonian can be analytically diagonalised, i.e. the eigenvalues E_j and eigenstates $|\psi_j\rangle$ of the stationary Schrödinger equation $H|\psi_j\rangle = E_j|\psi_j\rangle$ can be found

- ground state for $\gamma = 0$:

$$H_{\gamma=0} = -\sum_{k=1}^{L} \sigma_x^k$$

  - eigenvalues/-vectors of $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$$E_+ = 1 \quad \text{with } |e_+\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = |+\rangle = \frac{|\downarrow\rangle + |\uparrow\rangle}{\sqrt{2}}$$

$$E_- = -1 \quad \text{with } |e_-\rangle = \tfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = |-\rangle = \frac{-|\downarrow\rangle + |\uparrow\rangle}{\sqrt{2}}$$

- hence, the ground state of $H_{\gamma=0}$ is $|\psi_0\rangle_{\gamma=0} = |+\rangle_1 \otimes |+\rangle_2 \otimes \dots \otimes |+\rangle_L$, with energy $E_0^{\gamma=0} = -\sum_{k=1}^{L} E_+ = -L$

- the average magnetisation evaluates to

$$M = \frac{1}{L} {}_{\gamma=0}\langle\psi_0| \sum_{j=1}^{L} \sigma_z^j |\psi_0\rangle_{\gamma=0} = \frac{1}{L} L \langle + | \sigma_z | + \rangle$$

$$= \frac{1}{2}\Big(\underbrace{\langle\downarrow|\sigma_z|\downarrow\rangle}_{-1} + \underbrace{\langle\downarrow|\sigma_z|\uparrow\rangle}_{0} + \underbrace{\langle\uparrow|\sigma_z|\downarrow\rangle}_{0} + \underbrace{\langle\uparrow|\sigma_z|\uparrow\rangle}_{1}\Big) = 0$$

- for $\gamma = 0$ the ground state corresponds to a disordered phase with no net magnetisation
  ↳ corresponds to $T > T_c$

- ground state for $\gamma \gg 1$

$$H_{\gamma \gg 1} \approx -\gamma \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}$$

- eigenvalues/-vectors of σ_z

$E_\uparrow = 1$ with $|\uparrow\rangle = \binom{1}{0}$

$E_\downarrow = -1$ with $|\downarrow\rangle = \binom{0}{1}$

- there are two degenerate ground states of $H_{\gamma \gg 1}$ (consequence of so-called Z_2-symmetry)

$$\left.\begin{aligned} |\psi_{0\uparrow}\rangle_{\gamma \gg 1} &= |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes \dots \otimes |\uparrow\rangle_L \\ |\psi_{0\downarrow}\rangle_{\gamma \gg 1} &= |\downarrow\rangle_1 \otimes |\downarrow\rangle_2 \otimes \dots \otimes |\downarrow\rangle_L \end{aligned}\right\} E_0^{\gamma \gg 1} = -\gamma L$$

- the states have magnetisation ± 1, respectively
- for $\gamma \gg 1$ the ground state corresponds to ordered phase, analogous to $T < T_c$

Self-duality of quantum Ising model

- in order to find the critical point, i.e. the value of γ at which the transition between ordered and disordered phase takes place, the model does not need to be solved
- instead one can exploit the so-called self-duality property which establishes a relation between large and small γ-values
- starting point are the so-called domain-wall operators

  - $\mu_x^k = \sigma_z^k \sigma_z^{k+1}$; indicates presence of domain wall
  $$\mu_x^1 |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle = |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$$
  $$\mu_x^3 |\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle = -|\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$$
  - $\mu_z^k = \prod_{m=1}^{k-1} \sigma_x^m$; introduces a domain wall:
  $$\mu_z^4 |\downarrow\downarrow\downarrow\downarrow\downarrow\downarrow\rangle = |\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\rangle$$
- these operators obey the same (anti-) commutation relations as the Pauli matrices:

$\{\sigma_x, \sigma_z\} = 0$ $\qquad$ $\{\mu_x, \mu_z\} = 0$

$[\sigma_x^k, \sigma_z^m] = 0$ for $k \neq m$ $\qquad$ $[\mu_x^k, \mu_z^m] = 0$ for $k \neq m$

- in order to express H in terms of the domain-wall operators, we use that $\sigma_x^k = \mu_z^k \mu_z^{k+1}$

$$\hookrightarrow H = -\sum_{k=1}^{L} \mu_z^k \mu_z^{k+1} - \gamma \sum_{k=1}^{L} \mu_x^k$$

$$= \gamma \left(-\sum_{k=1}^{L} \mu_x^k - \gamma^{-1} \sum_{k=1}^{L} \mu_z^k \mu_z^{k+1} \right)$$

- since the σ's and μ's have the same algebra, this is a statement the symmetry of the spectrum:

$$H(\sigma; \gamma) = \gamma H(\mu; \tfrac{1}{\gamma}) \rightarrow E(\gamma) = \gamma\, E(\gamma^{-1})$$

- let us suppose now that there was a phase transition, i.e the two largest eigenvalues λ_1 and λ_2 of the transfer matrix become equal

- since $\lambda_1 = -\beta_{eff} \underset{\substack{\uparrow \\ \text{ground state} \\ \text{energy of H}}}{E_0(\gamma)}$ and $\lambda_2 = -\beta_{eff} \underset{\substack{\uparrow \\ \text{first excited} \\ \text{state energy of H}}}{E_1(\gamma)}$

this means $\underbrace{E_0(\gamma) = E_1(\gamma)}_{\text{ground state energy gap closes}}$

- however, this also means that

$$\gamma E_0(\gamma^{-1}) = \gamma E_1(\gamma^{-1}) \rightarrow E_0(\gamma^{-1}) = E_1(\gamma^{-1})$$

- assuming that there is only one value of γ where this happens, this must be at $\gamma = 1$

↳ the transition between the ordered and disordered phase takes place at the critical value $\gamma_c = 1$

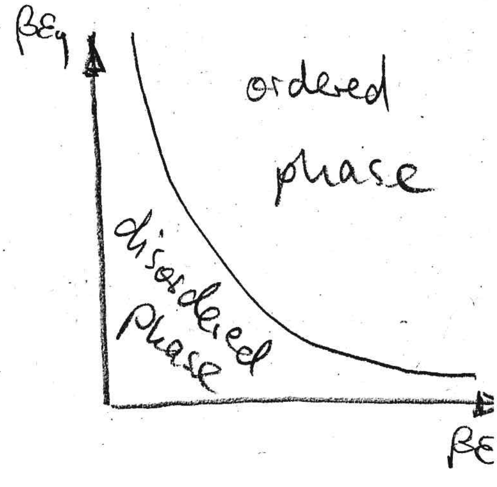
- relating this to the parameters of the classical 2d Ising model, we find

$$1 = \gamma_c = \beta_c \varepsilon_y e^{2\beta_c \varepsilon_x} \quad \text{with } \beta_c = \frac{1}{k_B T_c}$$

- this expression is the limiting case of the more general expression for the critical line

$$1 = \underbrace{\sinh(2\beta_c\varepsilon_x)}_{\xrightarrow[\beta_c\varepsilon_x \gg 1]{} \frac{e^{2\beta_c\varepsilon_x}}{2}} \underbrace{\sinh(2\beta_c\varepsilon_y)}_{\xrightarrow[\beta_c\varepsilon_y \ll 1]{} 2\beta_c\varepsilon_y}$$

which separates the ordered from the disordered phase



Exact solution of the quantum Ising model

- the quantum Ising model can be solved exactly by mapping the spins to fermions via the so-called Jordan-Wigner transformation
- the fermionic Hamiltonian can then be diagonalised via a so-called Bogoliubov transformation which yields an exact expression for the excitation spectrum
- Starting point is the Hamiltonian

$$H = -h \sum_{k=1}^{L} \sigma_x^k - \gamma \sum_{k=1}^{L} \sigma_z^k \sigma_z^{k+1}$$

- it is convenient to rotate the spin axis by $90°$ such that $\sigma_z^k \to \sigma_x^k$ and $\sigma_x^k \to -\sigma_z^k$
- moreover, we introduce the spin raising and lowering operators $\sigma_k^{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y)$

$\hookrightarrow$ $\sigma_x = \sigma^+ + \sigma^-$

- the Hamiltonian then becomes

$$H = +h \sum_{k=1}^{L} \sigma_z^k - \gamma \sum_{k=1}^{L} \sigma_x^k \sigma_x^{k+1}$$

$$= -h \sum_{k=1}^{L} (1 - 2\sigma_k^+ \sigma_k^-) - \gamma \sum_{k=1}^{L} \left(\sigma_k^+ \sigma_{k+1}^- + \sigma_k^- \sigma_{k+1}^+ + \sigma_k^+ \sigma_{k+1}^+ + \sigma_k^- \sigma_{k+1}^- \right)$$

- our goal is to bring the Hamiltonian into the form $H = \sum_k \varepsilon_k \eta_k^+ \eta_k$ where the η_k^+ / η_k are fermionic creation / annihilation operators
- the operator $\eta_k^+ \eta_k$ is the number operator, which can assume the values 0 or 1 and thus signals whether the k-th energy level / orbital is occupied or not
- the energy of the k-th state is ε_k
- it is tempting to identify the operators $\sigma_k^{\pm}$ somehow with the fermionic operators $\eta_k^{\pm}$
- this doesn't work, however, since the commutation relations are different:

spins fermions

$$\{\sigma_k^-, \sigma_k^+\} = 1 \ , \ [\sigma_k^-, \sigma_m^+] = 0 \quad \text{vs.} \quad \{c_k, c_k^+\} = 1 \ , \ \{c_k, c_m^+\} = 0$$

- i.e. fermion creation and annihilation operators anti-commute even when acting on different sites, while this is not the case for the spin operators

↳ spins on different sites „don't see" each other, while fermions have to „ensure" that the entire many-body wave function remains anti-symmetric when it is acted upon by operators

- we can relate the spin operators $\sigma_k^\pm$ to a set of fermionic operators, c_m / c_m^+ via the Jordan-Wigner transformation:

$$\sigma_k^+ = \left[\prod_{m=i}^{k-1} (1 - 2c_m^+ c_m)\right] c_k^+ = \exp\left[i\pi \sum_{m=1}^{k-1} c_m^+ c_m\right] c_k^+$$

$$\sigma_k^- = \left[\prod_{m=1}^{k-1} (1 - 2c_m^+ c_m)\right] c_k = \exp\left[-i\pi \sum_{m=1}^{k-1} c_m^+ c_m\right] c_k$$

$$= c_k \exp\left[-i\pi \sum_{m=1}^{k-1} c_m^+ c_m\right]$$

- the c-operators are fermionic:

$$\{c_k, c_m^+\} = \delta_{km} \quad , \quad \{c_k, c_m\} = \{c_k^+, c_m^+\} = 0$$

- the inverse transformation is

$$c_m = \left[\prod_{k=1}^{m-1} (1 - 2\sigma_k^+ \sigma_k^-) \right] \sigma_m^- = \left[\prod_{k=1}^{m-1} (-\sigma_z^k) \right] \sigma_m^-$$

$$c_m^+ = \left[\prod_{k=1}^{m-1} \sigma_z^k \right] \sigma_m^+$$

which can be used to show, that indeed the c-operators obey fermionic anti-commutation relations, given that the $\sigma_m^\pm$ are spin raising and lowering operators

- to express the Hamiltonian in terms of the fermionic operators, we use the following identities:

$$\sigma_k^+ \sigma_k^- = c_k^+ c_k$$

$$\sigma_k^+ \sigma_{k+1}^- = e^{i\pi \sum_{m=1}^{k-1} c_m^+ c_m} c_k^+ c_{k+1} e^{-i\pi \sum_{n=1}^{k} c_n^+ c_n}$$

$$= \underbrace{e^{i\pi \left(\sum_{m=1}^{k-1} c_m^+ c_m - \sum_{n=1}^{k-1} c_n^+ c_n \right)}}_{=1} c_k^+ e^{-i\pi c_k^+ c_k} c_{k+1}$$

$$= c_k^+ (1 - 2c_k^+ c_k) c_{k+1}$$

$$= c_k^+ c_{k+1} - 2 \underbrace{c_k^+ c_k^+}_{=0} c_k c_{k+1}$$

$$= c_k^+ c_{k+1}$$

- similarly, one finds

$$\sigma_k^- \sigma_{k+1}^+ = - c_k c_{k+1}^+ \ , \quad \sigma_k^+ \sigma_{k+1}^+ = c_k^+ c_{k+1}^+ \ , \quad \sigma_k^- \sigma_{k+1}^- = - c_k c_{k+1}$$

- putting everything together yields

$$H = -h \sum_{m=1}^{L} (1 - 2 c_m^+ c_m) - \gamma \sum_{m=1}^{L} \left(c_m^+ c_{m+1} + c_{m+1}^+ c_m + c_m^+ c_{m+1}^+ + c_{m+1} c_m \right)$$

- in the next step we introduce Fourier transformed fermionic operators

$$c_n = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} c_j e^{i \frac{2\pi}{L} n j} \quad \text{with } n = 1, \dots, L$$

- the inverse transform is $c_j = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} c_n e^{-i \frac{2\pi}{L} n j}$

- we can now write

$$\sum_{m=1}^{L} c_m^+ c_m = \frac{1}{L} \sum_{m n n'} c_n^+ c_{n'} e^{i \frac{2\pi}{L} n m} e^{-i \frac{2\pi}{L} n' m}$$

$$= \sum_{n n'} c_n^+ c_{n'} \underbrace{\frac{1}{L} \sum_{m=1}^{L} e^{i \frac{2\pi}{L} m (n - n')}}_{\delta_{n n'}} = \sum_{n n'} c_n^+ c_{n'} \delta_{n n'}$$

$$= \sum_{n=1}^{L} c_n^+ c_n$$

$$\sum_{m=1}^{L} c_m^+ c_{m+1} = \frac{1}{L} \sum_{m n n'} c_n^+ c_{n'} e^{i \frac{2\pi}{L} n m} e^{-i \frac{2\pi}{L} n' (m+1)} = \sum_{n n'} c_n^+ c_{n'} e^{-i \frac{2\pi}{L} n'} \delta_{n n'}$$

$$= \sum_{n} c_n^+ c_n e^{-i \frac{2\pi}{L} n}$$

$$\sum_{m=1}^{L} c_m^+ c_{m+1}^+ = \sum_{nn'} c_n^+ c_{n'}^+ e^{i\frac{2\pi}{L}n'} \underbrace{\frac{1}{L}\sum_m e^{i\frac{2\pi}{L}m(n+n')}}_{\delta_{n,-n'}}$$

- to make sense of the negative index, we relabel in the Fourier transform:

$$c_n = \frac{1}{\sqrt{L}}\sum_{j=1}^{L} c_j e^{i\frac{2\pi}{L}nj} \longrightarrow \frac{1}{\sqrt{L}}\sum_{j=-\frac{L}{2}}^{L/2} c_j e^{i\frac{2\pi}{L}nj}$$

$$\hookrightarrow \sum_{m=1}^{L} c_m^+ c_{m+1}^+ = \sum_{n=-\frac{L}{2}}^{L/2} c_n^+ c_{-n}^+ e^{-i\frac{2\pi}{L}n}$$

$$\sum_{m=1}^{L} c_m c_{m+1} = \sum_{n=-\frac{L}{2}}^{L/2} c_n c_{-n} e^{i\frac{2\pi}{L}n}$$

$$\sum_{m=1}^{L} c_{m+1}^+ c_m = \sum_{n=-\frac{L}{2}}^{L/2} c_n^+ c_n e^{i\frac{2\pi}{L}n}$$

- putting everything together, and introducing the momentum variable $q = \frac{2\pi}{L}n$, we can write the Hamiltonian as

$$H = \sum_q \Big[-h + 2h c_q^+ c_q - \gamma \underbrace{(e^{-iq} + e^{iq})}_{2\cos q} c_q^+ c_q - \gamma e^{-iq} c_q^+ c_{-q}^+ - \gamma e^{iq} c_q c_{-q}\Big]$$

$$= \sum_q \Big[-h - 2(h-\gamma\cos q) c_q^+ c_q - \frac{1}{2}\gamma\left(e^{-iq} c_q^+ c_{-q}^+ + e^{iq} c_{-q}^+ c_q^+\right)$$

$$- \frac{1}{2}\gamma\underbrace{\left(e^{iq} c_q c_{-q} + e^{-iq} c_{-q} c_q\right)}_{(-e^{iq}+e^{-iq})\, c_{-q} c_q \,=\, -2i\sin(q)\, c_{-q} c_q}\Big]$$

changing order of summation

$\hookrightarrow H = \sum_q \left[-h + 2(h - \gamma\cos q)\, c_q^\dagger c_q + i\gamma \sin q \,(c_{-q}^\dagger c_q^\dagger + c_{-q} c_q) \right]$

- this Hamiltonian couples only the momenta q and $-q$
- this coupling can be removed by applying a so-called Bogoliubov transformation, which introduces the new fermionic operators

$$\eta_q = u_q c_q - i v_q c_{-q}^\dagger$$

with u_q and v_q being real numbers, satisfying: $u_q^2 + v_q^2 = 1$, $u_{-q} = u_q$, $v_{-q} = -v_q$ (these constraints ensure fermionic commutation relations)

- given these constraints a convenient paramterisation is $u_q = \cos(\frac{\theta_q}{2})$, $v_q = \sin(\frac{\theta_q}{2})$
- we can now express the Hamiltonian in terms of these new fermions using the inverse Bogoliubov transformation

$$c_q = u_q \eta_q + i v_q \eta_{-q}^\dagger$$

• this is done by rewriting the Hamiltonian as

$$H = -Lh + \sum_q (h - \gamma \cos q)\left(c_q^{+} c_q - c_{-q} c_{-q}^{+}\right)$$

$$+ i\gamma \sum_q \sin q \left(-c_q^{+} c_{-q}^{+} + c_{-q} c_q\right)$$

$$= -Lh + \sum_q \begin{pmatrix} c_q^{+} \\ c_{-q} \end{pmatrix}^{T} \begin{pmatrix} h - \gamma\cos q & -i\gamma \sin q \\ i\gamma \sin q & -h + \gamma \cos q \end{pmatrix} \begin{pmatrix} c_q \\ c_{-q}^{+} \end{pmatrix}$$

• introducing the η-operators via

$$\begin{pmatrix} c_q \\ c_{-q}^{+} \end{pmatrix} = \begin{pmatrix} \cos\frac{\theta_q}{2} & i\sin\frac{\theta_q}{2} \\ i\sin\frac{\theta_q}{2} & \cos\frac{\theta_q}{2} \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^{+} \end{pmatrix}$$ we can write

$$H = -Lh + \sum_q \begin{pmatrix} \eta_q^{+} \\ \eta_{-q} \end{pmatrix} \begin{pmatrix} \cos\frac{\theta_q}{2} & -i\sin\frac{\theta_q}{2} \\ -i\sin\frac{\theta_q}{2} & \cos\frac{\theta_q}{2} \end{pmatrix} \begin{pmatrix} h - \gamma\cos q & -i\gamma\sin q \\ i\gamma\sin q & -h+\gamma\cos q \end{pmatrix} \begin{pmatrix} \cos\frac{\theta_q}{2} & i\sin\frac{\theta_q}{2} \\ i\sin\frac{\theta_q}{2} & \cos\frac{\theta_q}{2} \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^{+} \end{pmatrix}$$

$$= -Lh + \sum_q \begin{pmatrix} \eta_q^{+} \\ \eta_{-q} \end{pmatrix} \begin{pmatrix} h\cos\theta_q - \gamma\cos(q+\theta_q) & i\left(h\sin\theta_q - \gamma\sin(q+\theta_q)\right) \\ -i\left(h\sin\theta_q - \gamma\sin(q+\theta_q)\right) & -h\cos\theta_q + \gamma\cos(q+\theta_q) \end{pmatrix} \begin{pmatrix} \eta_q \\ \eta_{-q}^{+} \end{pmatrix}$$

• the matrix becomes diagonal, when

$$h\sin\theta_q - \gamma\sin(q+\theta_q) = 0 \rightarrow \tan\theta_q = \frac{\gamma\sin q}{h - \gamma\cos q}$$

• here $h\cos\theta_q - \gamma\cos(q+\theta_q) = \sqrt{\gamma^2 + h^2 - 2h\gamma\cos q}$

- hence

$$H = -Lh + \sum_q \sqrt{\gamma^2 + h^2 - 2h\gamma\cos q}\,\left(\eta_q^+\eta_q - \eta_{-q}\eta_{-q}^+\right)$$

- using $\eta_{-q}\eta_{-q}^+ = 1 - \eta_{-q}^+\eta_{-q}$ and $\cos(-q) = \cos(q)$

the Hamiltonian finally reads

$$H = \sum_q \varepsilon_q \eta_q^+ \eta_q + \overbrace{\sum_q \varepsilon_q - Lh}^{\text{we neglect this constant term in the following}}$$

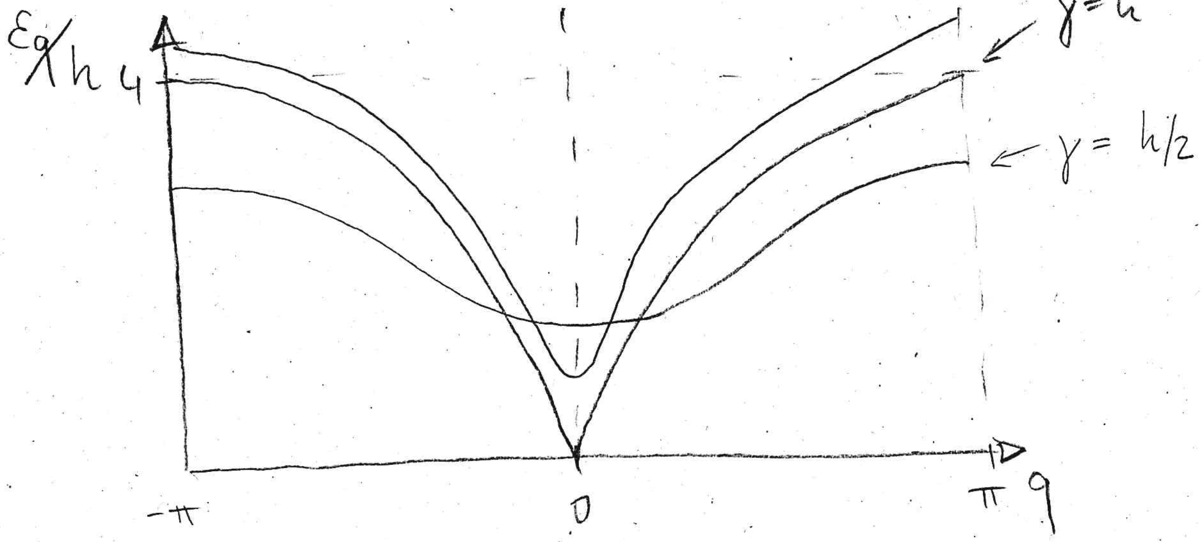
with the energies $\varepsilon_q = 2\sqrt{\gamma^2 + h^2 - 2h\gamma\cos q}$

- the ground state of this Hamiltonian is given by the state $|0\rangle$ with $\eta_q|0\rangle = 0$
- this is the vacuum state and all higher lying states contain at least one fermion
- the energies ε_q are all positive
- hence the first excited state is $\eta_{q=0}^+|0\rangle$ and its energy is

$$\underset{\substack{\uparrow \\ \text{energy gap}}}{\varepsilon_0} = 2\sqrt{\gamma^2 + h^2 - 2h\gamma} = 2|\gamma - h|$$

- the energy gap is closing to zero at $\gamma = h$, i.e. $\frac{\gamma}{h} = 1$
- here the transition between the ordered and disordered state takes place

excitation spectrum



- at the critical point the dispersion relation behaves as $\mathcal{E}_q \sim |q|$ for small q
- away from criticality one finds $\mathcal{E}_q \sim q^2$

↳ dynamical behaviour of excitations is markedly different (relativistic vs. massive quasi-particles)