Advanced Statistical Physics

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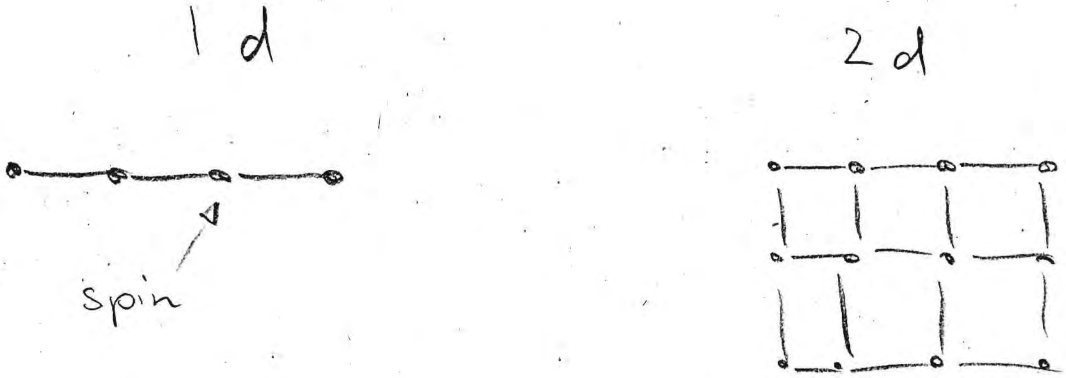
The Ising model

- 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

$$Z = \mathrm{Tr}\, e^{-\beta E} = \sum_{S_1=\pm 1} \dots \sum_{S_N=\pm 1} e^{\beta \varepsilon \sum_{i=1}^{N} S_i S_{i+1} + \beta H \sum_{i=1}^{N} S_i}$$

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

$$Z = \sum_{S_1} \dots \sum_{S_N} \underbrace{\left[e^{\frac{h}{2}(S_1+S_2)+KS_1S_2}\right]}_{T_{S_1S_2}} \times \underbrace{\left[e^{\frac{h}{2}(S_2+S_3)+KS_2S_3}\right]}_{T_{S_2S_3}} \times \dots \times \underbrace{\left[e^{\frac{h}{2}(S_N+S_1)+KS_NS_1}\right]}_{T_{S_NS_1}}$$

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

$$T_{S_1S_2} = e^{\frac{h}{2}(S_1+S_2)+KS_1S_2}$$

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

- the partition function then becomes

$$Z = \sum_{S_1} \dots \sum_{S_N} T_{S_1S_2} T_{S_2S_3} \dots T_{S_NS_1}$$

- T is called the transfer matrix

(5)

- 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 $\beta = 1/k_BT$)

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

Thermodynamic properties of the 1d Ising model

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

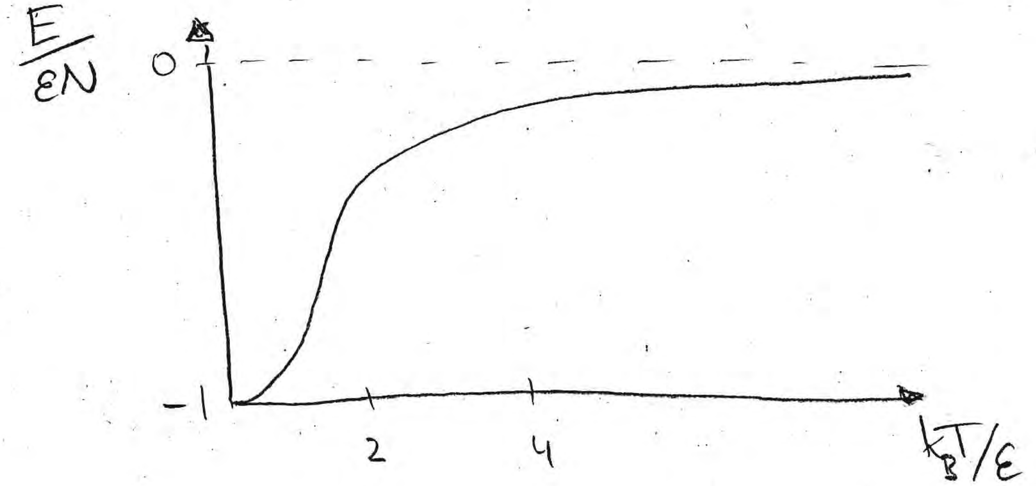
$$\frac{F}{N} = \underbrace{-\varepsilon}_{\substack{\text{energetic part;}\\ \text{dominates @ } T\to 0\\ (\beta\to\infty)}} - \underbrace{\frac{1}{\beta}\log\left(1 + e^{-2\beta\varepsilon}\right)}_{\substack{\text{entropic part;}\\ \text{dominates @ } T\to\infty\\ (\beta\to 0)}}$$

$$F = E - TS$$

- internal energy:

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

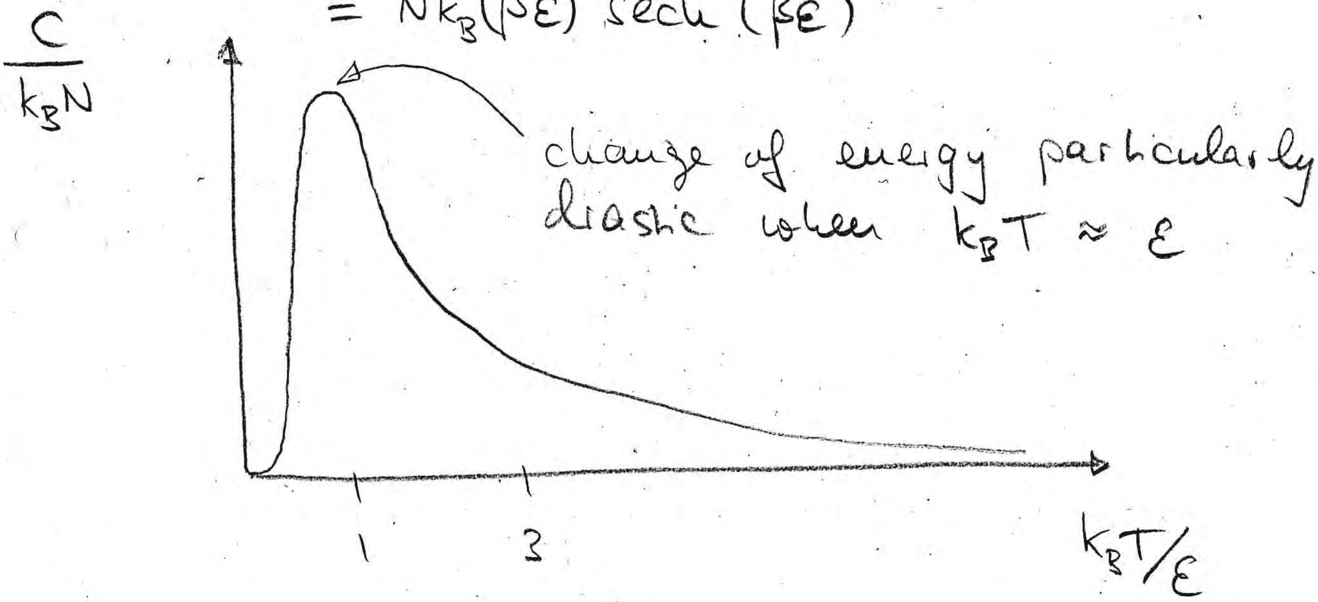
$$= -N\frac{\partial}{\partial\beta}\log 2\cosh(\beta\varepsilon) = -N\varepsilon\tanh(\beta\varepsilon)$$



- specific heat:

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

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

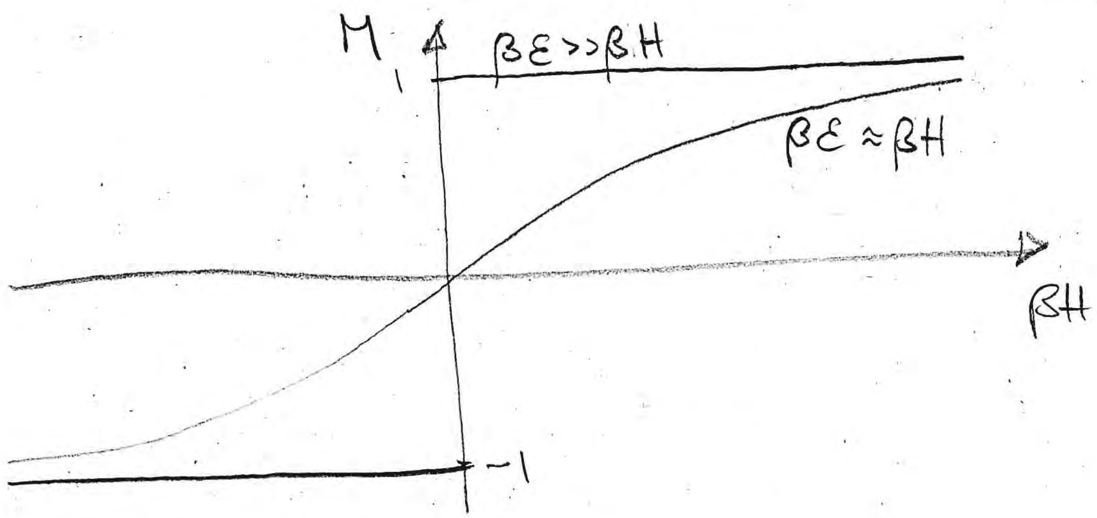


- peak is the so-called Schottky anomaly
- characteristic for systems with discrete energy levels

• 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 $\beta\varepsilon >> \beta H$ 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 $\beta\varepsilon >> 1$ and βH finite
(T goes to zero and H changes in a way that H/T remains finite)

- here we can write

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

and hence

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

- the free energy then becomes

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

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:

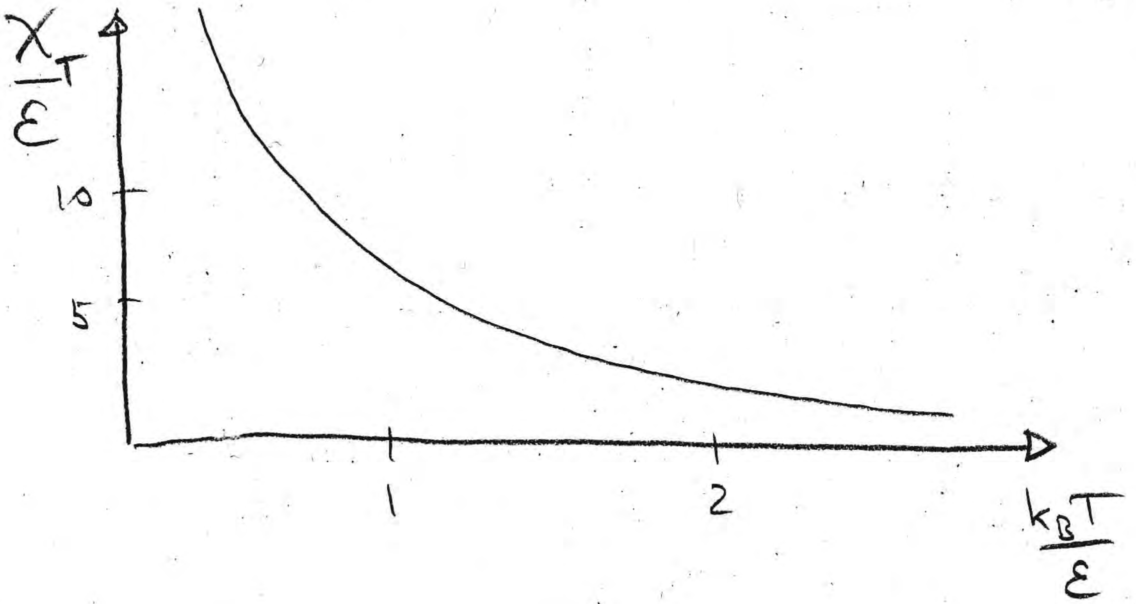
- describes how magnetisation changes in response to a magnetic field

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

- 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

$$\langle s_i \rangle = \frac{1}{Z} \sum_{s_1} \dots \sum_{s_N} e^{-\beta E} s_i$$

$$= \frac{1}{Z} \sum_{s_1} \dots \sum_{s_N} T_{s_1 s_2} T_{s_2 s_3} \dots T_{s_{i-1} s_i} \, s_i \, T_{s_i s_{i+1}}$$

- 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

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

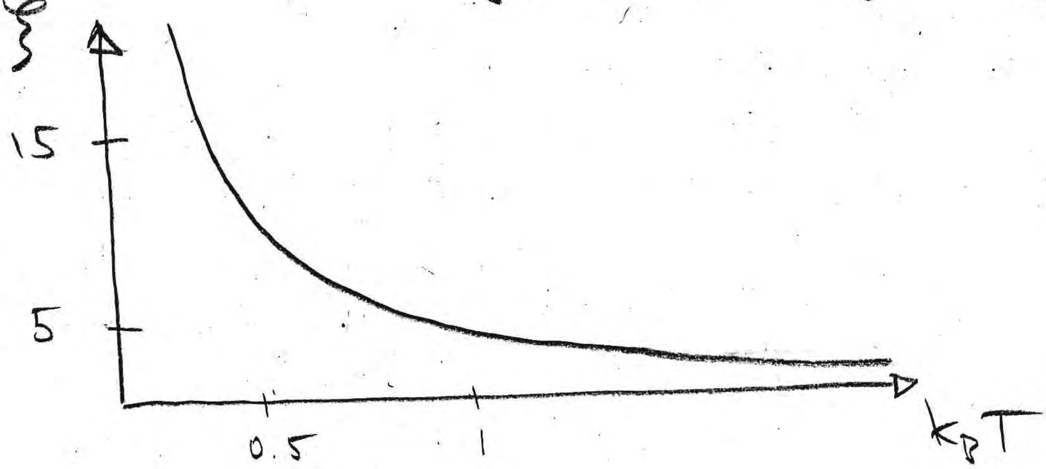
$$= \alpha_3 \alpha_4 \, e^{-j/\xi}$$

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. $T \to 0$

  $\hookrightarrow$ 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:

  ↳ $F_{\uparrow\uparrow\downarrow\downarrow} = -N\varepsilon + 2\varepsilon - TS$

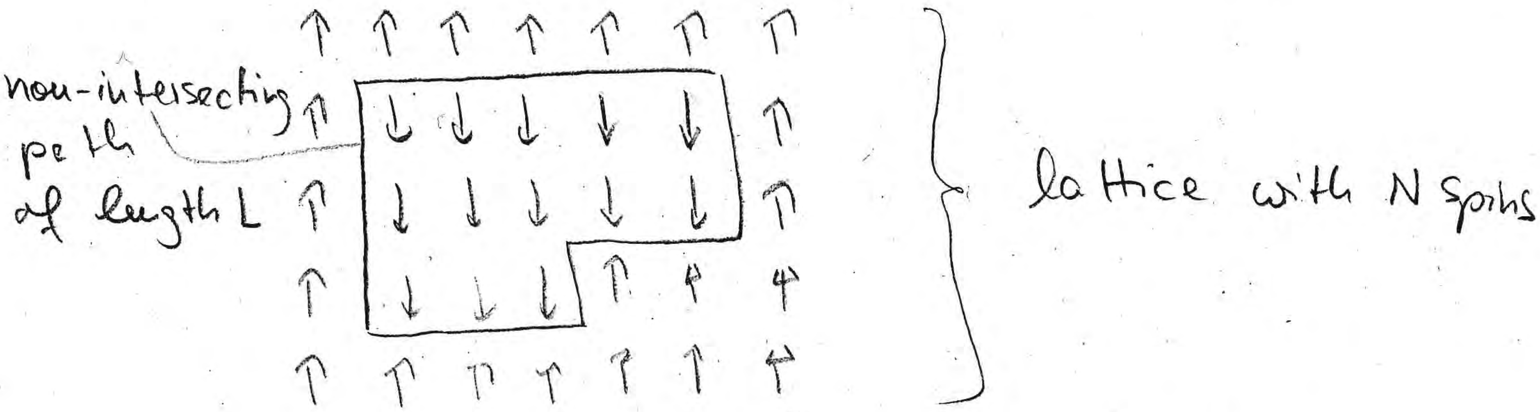
↳ $\Delta F = F_{\uparrow\uparrow\downarrow\downarrow} - F_{\uparrow\uparrow\uparrow\uparrow} = 2\varepsilon - k_B T \log N$

↳ 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

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

$$\approx -\varepsilon \sum_{\langle ij \rangle} S_i \underbrace{M}_{} = -\varepsilon \underbrace{2d}_{} M \sum_i S_i$$

magnetisation, assuming that system is homogeneous

coordination number: 2× dimension for hypercubic lattice

- the mean field energy is thus

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

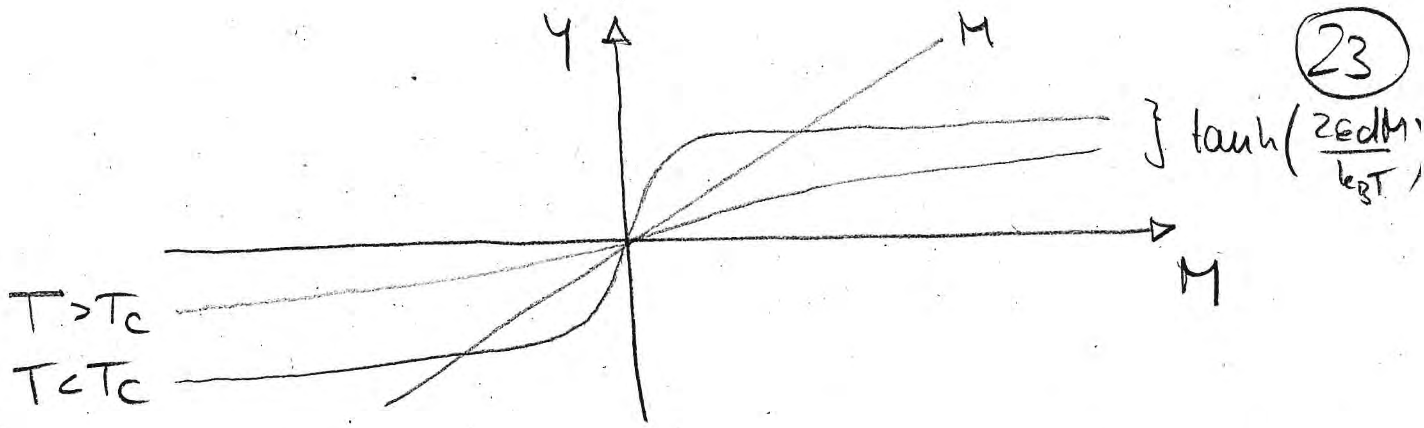
$$= -(H + 2\varepsilon d M) \sum_i S_i$$

- 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

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

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

- 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

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

- 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

$$\overset{\text{assuming translation invariance}}{=} \frac{1}{k_BT}\sum_j G_{ij} \approx \frac{1}{k_BT a^d}\int d^d r\, G(r)$$

a: 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 $T=0$)

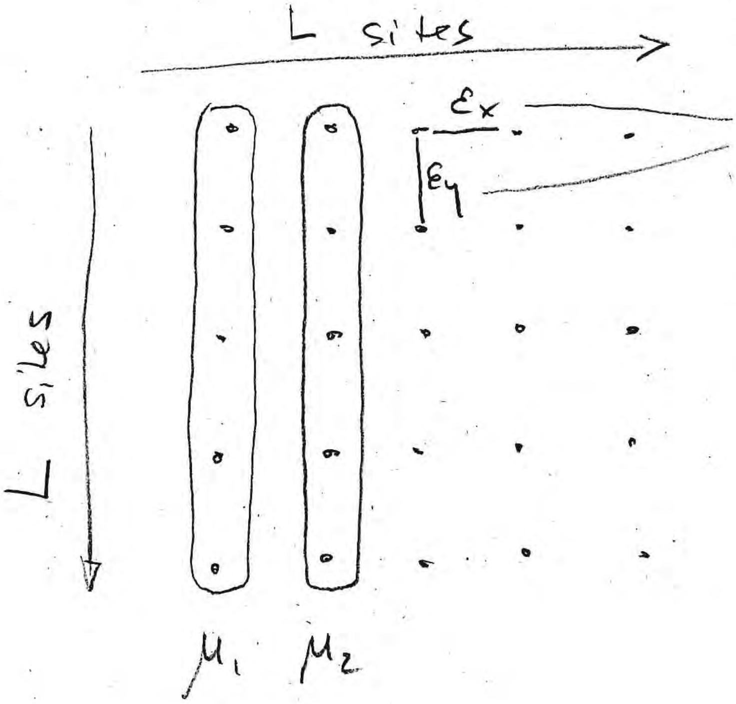
↳ generally a diverging χ_T signals a diverging correlation length

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 condition



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

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

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

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

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

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

- one thus finds that

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

- 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, $\varepsilon_x = \varepsilon_y$

- free energy per spin:

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

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

- energy per spin:

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

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

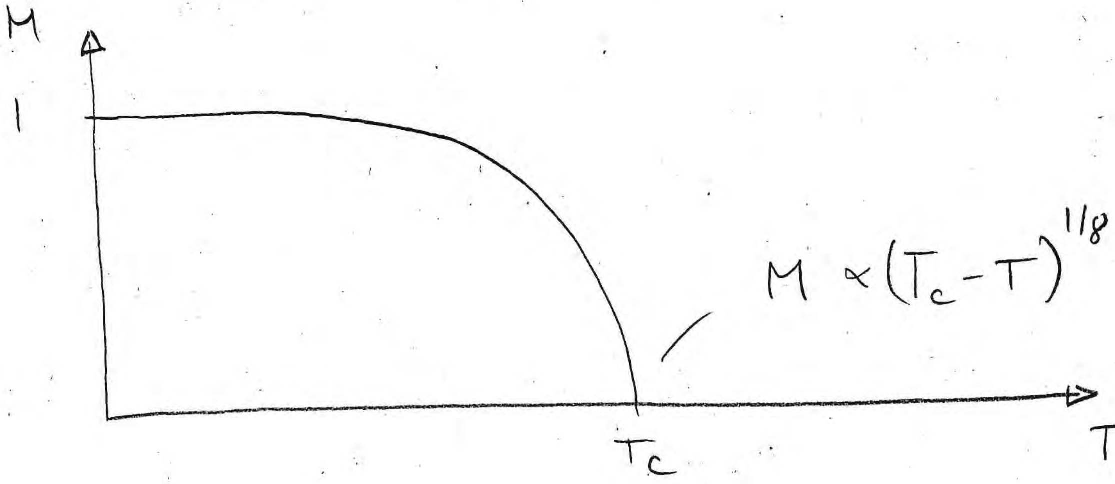
- $K_1(k)$ has a singularity at $k=1$, which determines the critical temperature

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

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

- magnetisation:

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



- 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: $e^x \approx 1 + x \ldots$

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

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

- 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

$$M = \frac{1}{L}\langle\psi_0|\sum_{j=1}^{L}\sigma_z^j|\psi_0\rangle_{\gamma=0} = \frac{1}{L}\, L\,\langle +|\sigma_z|+\rangle$$
$$= \frac{1}{2}\Big(\underbrace{\langle\downarrow|\sigma_z|\downarrow\rangle}_{-1} + \underbrace{\langle\downarrow|\sigma_z|\uparrow\rangle}_{0} + \underbrace{\langle\uparrow|\sigma_z|\downarrow\rangle}_{0} + \underbrace{\langle\uparrow|\sigma_z|\uparrow\rangle}_{1}\Big) = 0$$

- 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

$$E_\uparrow = 1 \quad \text{with } |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$E_\downarrow = -1 \quad \text{with } |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- there are two degenerate ground states of $H_{\gamma\gg 1}$ (consequence of so-called $\mathbb{Z}_2$-symmetry)

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

- 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:

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

$[\sigma_x^k, \sigma_z^m] = 0$ 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:

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

- 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 $\gamma_c = 1$

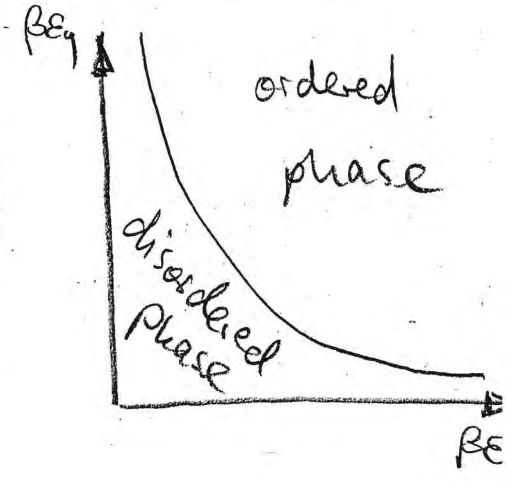
- relating this to the parameters of the classical 2d Ising model, we find

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

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

$$1 = \sinh(2\beta_c\varepsilon_x)\,\sinh(2\beta_c\varepsilon_y)$$

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



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:

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

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

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

- 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

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

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

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:

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

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

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

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

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

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

- 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

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

- in the next step we introduce Fourier transformed fermionic operators

$$\tilde{c}_n = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} c_j e^{i \frac{2\pi}{L} n j} \quad \text{with } n = 1, \ldots, L$$

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

- we can now write

$$\sum_{m=1}^{L} c_m^+ c_m = \frac{1}{L} \sum_{m n n'} \tilde{c}_n^+ \tilde{c}_{n'} e^{i \frac{2\pi}{L} n m} e^{-i \frac{2\pi}{L} n' m}$$

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

$$= \sum_{n=1}^{L} \tilde{c}_n^+ \tilde{c}_n$$

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

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

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

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

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

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

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

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

- 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

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

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

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

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- this is done by rewriting the Hamiltonian as

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

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

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

- 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

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

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

- 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

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

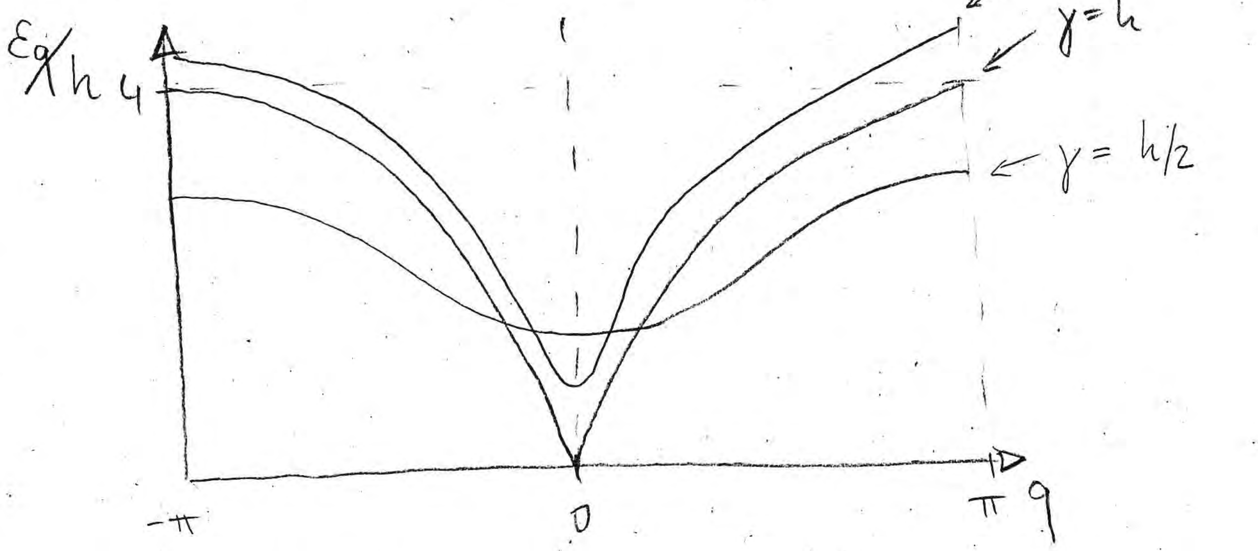
with the energies $\varepsilon_q = 2\sqrt{\gamma^2 + h^2 - 2h\gamma\cos q}$

- 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 $\varepsilon_q \sim |q|$ for small q
- away from criticality one finds $\varepsilon_q \sim q^2$

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

Landau approach to phase transitions

Order parameter

- the Ising model exhibits a phase transition at T_c
- below T_c the magnetisation M is finite, while above T_c, i.e. in the disordered (symmetric) phase, it is zero
- apparently M is a quantity that signals when a magnet is in the ordered (symmetry-broken) phase
- this concept can be generalised and leads to the notion <u>order parameter</u>
- the order parameter is typically an extensive thermodynamic quantity, which is accessible by measurements

- when the order parameter changes, work is done on the system:

$$dW = H \, dM$$

- here H (which is the magnetic field strength) represents the so-called "<u>conjugate field</u>"

- order parameters don't have to be scalars, e.g. in the Heisenberg model with Hamiltonian

$$\mathcal{H}(\{\vec{S}_i\}) = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

the order parameter is the magnetisation vector:

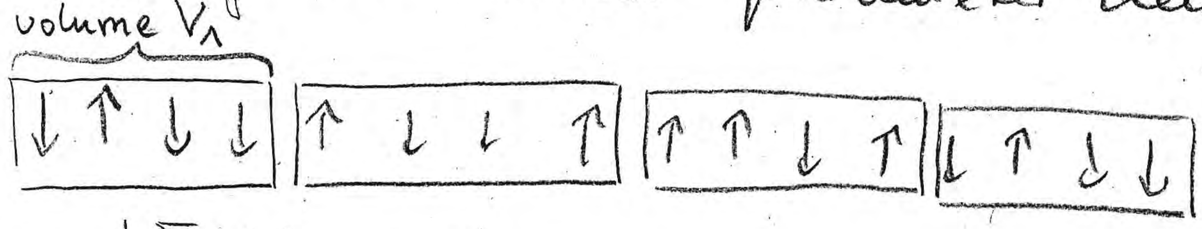
$$\vec{M} = \sum_i \langle \vec{S}_i \rangle = \begin{cases} \vec{0} \, ; & T > T_c \\ M \hat{n} \, ; & T < T_c \end{cases}$$

unit vector pointing in arbitrary direction (higher symmetry than Ising model,

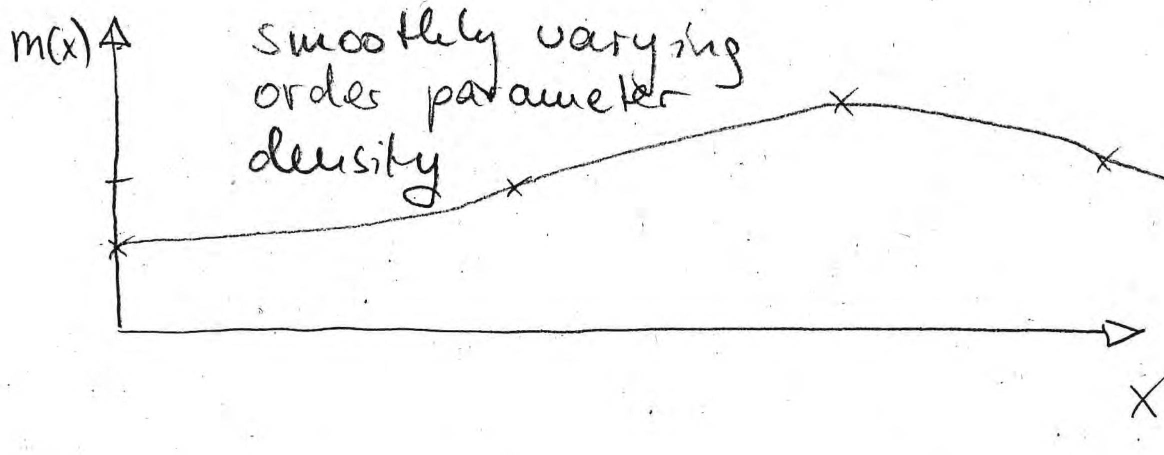
- Landau's theory of phase transition is built on the concept of the order parameter

- it establishes a connection between the order parameter density and the partition function

- the idea is to perform a coarse graining procedure that removes microscopic details and permits to express the partition function in terms of the order parameter density



$m(x_1) = \frac{1}{V_\Lambda} \sum_j \langle S_j \rangle$ $\quad m(x_2) \quad m(x_3) \quad m(x_4)$



- at the level of the partition function this looks as follows

$$Z = \sum_{\{S_i\}} e^{-\beta \overbrace{H}^{\text{Hamiltonian}}(\{S_i\})} = \sum_{m(x_i)} \sum_{\{\bar{S}\}} e^{-\beta H(\{S_i\})}$$

$\sum_{\{S_i\}}$: sum over all spin configurations

$\sum_{m(x_i)}$: sum over all possible values of the local magnetisation density

$\sum_{\{\bar{S}\}}$: sum over all microscopic configurations leading to a magnetisation density $m(x_i)$

$$= \sum_{m(x)} e^{-\beta L(\{m(x)\})} \left(= e^{-\beta G(H,T)} \right)$$

$G(H,T)$: notion typically used for magnetic systems → (Gibbs) free energy

- the quantity $L(\{m(x)\})$ is referred to as „Landau free energy"
- usually, L is written down in a phenomenological way, and its structure is dictated by the symmetries of the underlying system

- to illustrate the idea behind the construction of L, lets consider the mean field equation of the Ising magnet:

$$\frac{H}{k_B T} = M\left(1 - \frac{T_c}{T}\right) + M^3\left(\frac{T_c}{T} - \left(\frac{T_c}{T}\right)^2 + \frac{1}{3}\left(\frac{T_c}{T}\right)^3 + \dots\right)$$

- denoting the order parameter as $\eta = M$ and introducing the abbreviation $t = \frac{T - T_c}{T_c} = \frac{1}{\tau} - 1$ this becomes (using $\tau = \frac{1}{1+t} \approx 1 - t + \dots$)

$$\frac{H}{k_B T} = \eta t + \eta^3 + \underbrace{\mathcal{O}(t\eta^3)}_{\substack{\text{negligible near } T_c \\ \text{where } |t|, \eta \ll 1}}$$

- the idea is now to interpret this equation as the result of a saddle point approximation to the partition function:

$$\sum_{m(x)} e^{-\beta L(\{m(x)\})} \approx e^{-\min_{m(x)} \left[\beta L(\{m(x)\})\right]}$$

↳ in thermal equilibrium the system „chooses" the order parameter such that it minimises the Landau free energy

- in the current example, the magnetisation η, given H and T, in equilibrium is $\frac{H}{k_B T} = \eta t + \eta^3$

- this result is also obtained from the saddle point approximation

$$\sum_{\eta} e^{-\beta L(\eta)} \approx e^{-\min_{\eta} \beta L(\eta)},$$

when choosing the Landau free energy to be

$$L(H,T,\eta) = L_0(H,T) - \frac{\eta H}{k_B T} + \frac{t\eta^2}{2} + \frac{1}{4}\eta^4$$

$$\hookrightarrow \; 0 = \frac{\partial L(H,T,\eta)}{\partial \eta} = -\frac{H}{k_B T} + \eta t + \eta^3$$

- Landau theory postulates that such Landau free energy L, can be generically written down for an order parameter density η

(1) L has to be consistent with the symmetries of the system

(2) Near the critical temperature T_c, L can be expanded in a power-series in η. Introducing the Landau free energy density $\mathcal{L} = \frac{L}{V}$ this means:

$$\mathcal{L} = \sum_{n=0}^{\infty} \underbrace{a_n}_{\text{numerical coefficients}} (\underbrace{[K]}_{\substack{\text{coupling constants} \\ (H, J, T)}}) \, \eta^n$$

(3) In a spatially inhomogeneous system, with a spatially varying order parameter, i.e. $\eta(\vec{r})$, $\mathcal{L}$ is a local function, meaning that $\mathcal{L}$ depends only on a finite number of spatial derivatives.

(4) In the disordered (symmetric) phase of the system, the order parameter is 0, while it is small but non-zero in the ordered (symmetry-broken) phase.
↳ $\mathcal{L}$ has to be constructed accordingly.

Landau theory of a ferromagnet (and a van-der-Waals gas)

- we construct now, using the above principles, the Landau free energy of a ferromagnet
- it turns out that the resulting phenomenology, i.e. phases and phase transitions, is the same as for the van-der-Waals gas
  ↳ this is a hint towards the concept of universality, i.e. the fact that different physical systems behave in the „same way" near critical points

- we consider a ferromagnet in the absence of external fields

$$\mathcal{L} = a_0 + a_1 \eta + a_2 \eta^2 + a_3 \eta^3 + a_4 \eta^4 + \dots$$

unimportant constant that can be set to zero

terms are forbidden by symmetry, because the energy function of a ferromagnet is invariant under $s_i \to -s_i$, i.e. $\mathcal{L}$ has to be invariant under $\eta \to -\eta$

$\hookrightarrow$ $$\mathcal{L} = a_2 \eta^2 + a_4 \eta^4$$

- we write now $a_2 = a_2^0 + t\, a_2' + \dots$ $\quad t = \frac{T - T_c}{T}$

and require that $\left\{ \begin{array}{l} \eta = 0 \text{ for } T > T_c \\ \eta \neq 0 \text{ for } T < T_c \end{array} \right\}$ and

- solving $0 \stackrel{!}{=} \frac{\partial \mathcal{L}}{\partial \eta} = 2 a_2 \eta + 4 a_4 \eta^3$

yields $\eta = 0$ or $\eta = \sqrt{\frac{-a_2}{2a_4}}$

- in order for η to be non-zero when $T < T_c$, i.e. $t < 0$, one has to choose $a_2 = \underbrace{a_2^0}_{=0} + t a_2^1$

- the coefficient a_4 can be chosen to be independent of T, since all the requirement of the Landau construction (points (1) - (4)) are met by this choice

- to account for a magnetic field, we have to add a symmetry breaking term (a term that is not invariant under $\eta \to -\eta$)
- the simplest choice is $-H\eta$, such that the Landau free energy density reads

$$\mathcal{L} = a t \eta^2 + \frac{1}{2} b \eta^4 - H\eta$$

- we will show now how Landau theory accounts for phase transitions and especially for non-analytic behaviour near T_c

- we first discuss the case of the <u>continuous phase transition</u> that occurs when $H = 0$

- for $T > T_c$ the minimum of $\mathcal{L}$ is at $\eta = 0$

- also at $T = T_c$ the minimum of $\mathcal{L}$ is at $\eta = 0$, but in this case also the curvature of $\mathcal{L}$ is 0 at $\eta = 0$.

- for $T < T_c$, $\mathcal{L}$ has two degenerate minima, which occur at

$$\eta = \pm \eta_s(T) = \pm \sqrt{-\frac{at}{b}}$$

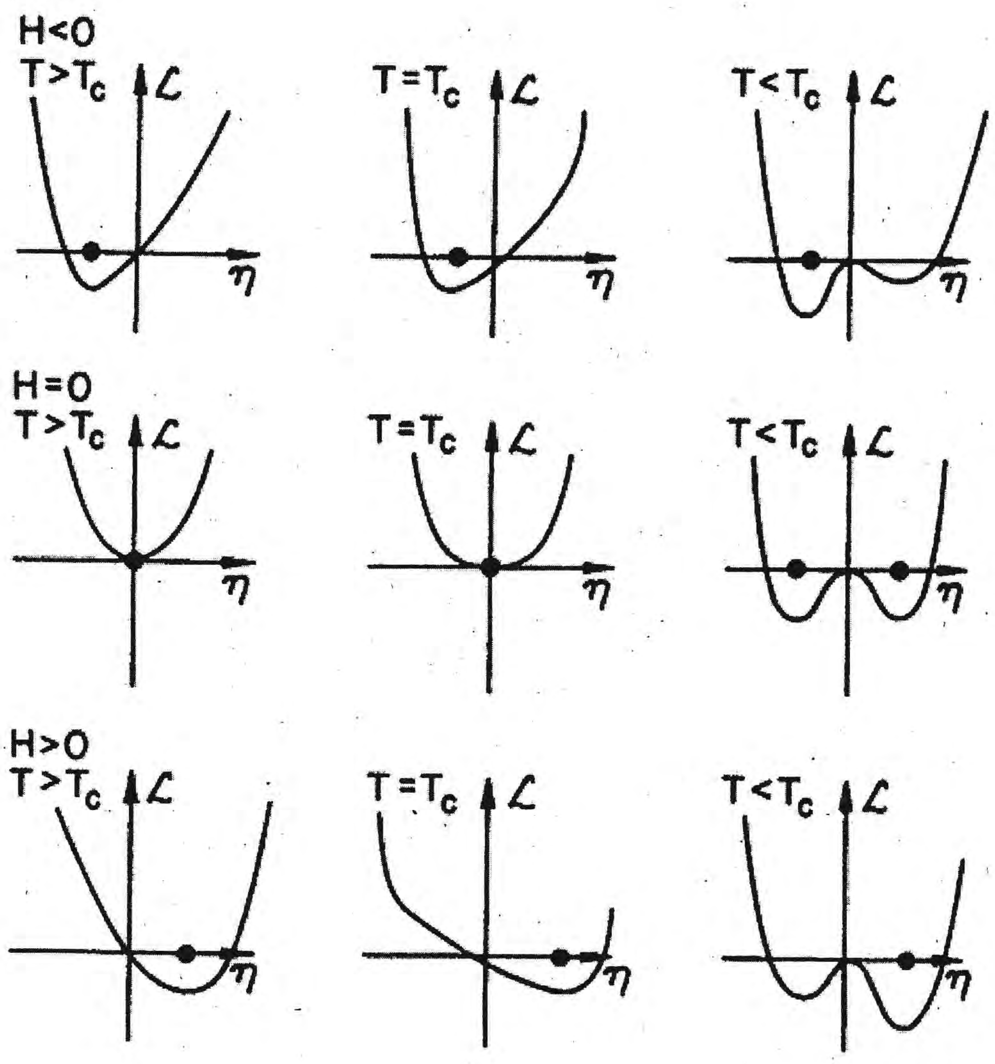


Figure 5.1 The Landau free energy density for various values of T and H. The • indicates the value of η at which $\mathcal{L}$ achieves its global minimum. The right-most column of graphs depicts the first order transition, which occurs for $T < T_c$ as H is varied from a negative to a positive value. The central row depicts the continuous transition, which occurs for $H = 0$ as T is varied from above T_c to below T_c.

Nigel Goldenfeld
Lectures on Phase Transitions and Renormalization Group
CRC Press (1992)

- the last expression allows to extract already one critical exponent from Landau theory

$$\eta_s(T) \propto |T-T_c|^\beta \rightarrow \beta = 1/2$$

- another critical exponent (denoted as α) can be extracted from the behaviour of the heat capacity C_V near T_c, which is defined as $C_V = T\left(\frac{\partial S}{\partial T}\right)_V$

- using the connection between entropy and (Gibbs) free energy, $S = -\frac{\partial G}{\partial T}$, this amounts to

$$C_V = -T\frac{\partial^2 G}{\partial T^2}$$

- to connect this to the Landau free energy, we remember, that

$$e^{-\beta G} \approx e^{-\min_\eta \beta V \mathcal{L}(\{\eta\})}$$

- hence, we can evaluate G from the value that $\mathcal{L}$ assumes at its minimum

- using that for $t>0$ the minimum value is $\mathcal{L}_{min}=0$, and at $t<0$ the minimum value is $\mathcal{L}_{min} = -\frac{1}{2}\frac{a^2 t^2}{b}$, one finds

$$C_V \propto \begin{cases} 0 & , \quad T > T_c \\ T_c \frac{a^2}{b} & , \quad T < T_c \end{cases}$$

$$\hookrightarrow \quad C_V \propto |T-T_c|^{\alpha} \quad \rightarrow \quad \alpha = 0$$

- to compute the remaining exponents, we differentiate $\mathcal{L}$ with respect to H, yielding $at\eta + b\eta^3 = \frac{1}{2}H \quad (*)$
- at the critical point $(t=0)$ this yields $\eta \propto H^{1/\delta} \longrightarrow \delta = 3$
- next, we calculate the isothermal susceptibility:

$$\chi_T(H) = \left(\frac{\partial \eta(H)}{\partial H}\right)_T = \frac{1}{2(at + 3b\,\eta^*(H)^2)}$$

solution of $(*)$

- we are interested in calculating χ_T in the limit $H \to 0$
- for $t > 0$ $(T > T_c)$, $\eta^*(H \to 0) = 0$

  ↳ $\chi_T = \frac{1}{2at} \propto |T - T_c|^{-\gamma} \to \gamma = 1$
- for $t < 0$ $(T < T_c)$, $\eta^*(H \to 0) = \pm\sqrt{\frac{-at}{b}}$

  ↳ $\chi_T = \frac{1}{-4at} \propto |T - T_c|^{-\gamma'} \to \gamma' = 1$

↳ we recovered all mean field exponents, but as we will see later Landau theory can deliver more, e.g. the critical exponent related to spatial correlations

- let us now consider a Landau free energy of the form

$$\mathcal{L} = a t \eta^2 + \frac{1}{2} b \eta^4 + C \eta^3 ,$$

which contains a cubic term, unlike the Landau free energy of the Ising model

- this $\mathcal{L}$ gives rise to a so-called <u>first order phase transition</u>:

- the extremal values of $\mathcal{L}$ are either at $\eta_1 = 0$ or at $\eta_2 = -c \pm \sqrt{c^2 - \frac{at}{b}}$, with $c = \frac{3C}{4b}$

- the solution η_2 becomes acceptable when $c^2 - \frac{at}{b} > 0$, i.e. when $t < t^* = \frac{bc^2}{a}$

- for $t < t^*$ $\mathcal{L}$ develops a second local minimum, in addition to the one at η_1

- at a certain temperature t_1 the value of $\mathcal{L}$ at η_1 becomes equal to the value of $\mathcal{L}$ at η_2

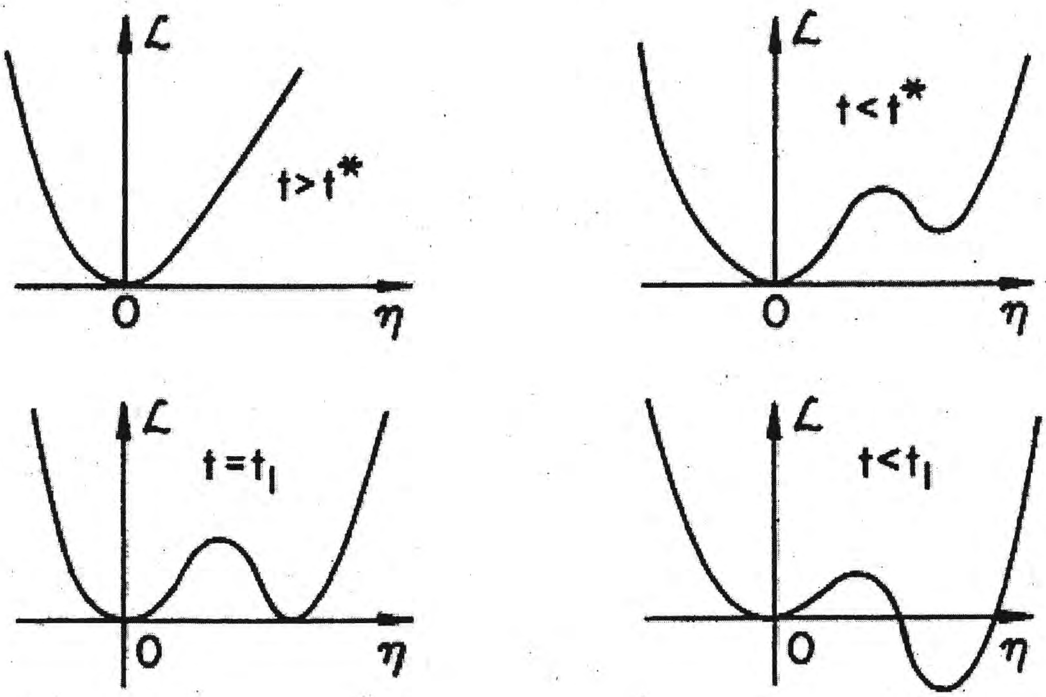


Figure 5.2 $\mathcal{L}$ as a function of η for various temperatures, showing the Landau theory description of a first order transition.

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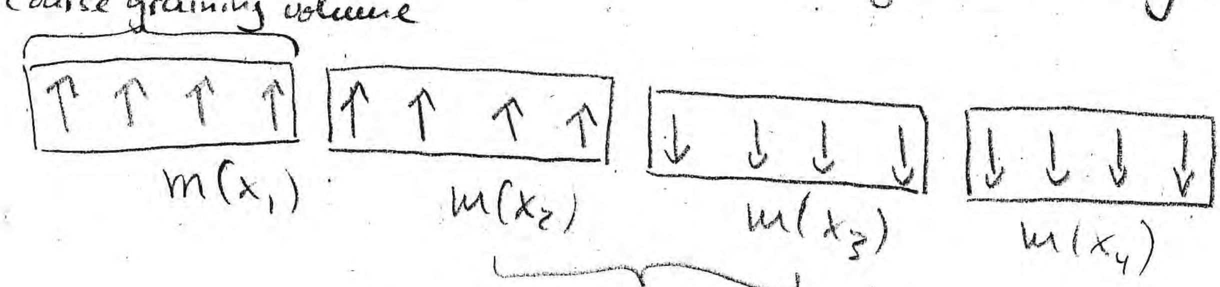
CRC Press (1992)

- when t is lowered below t_1, $\mathcal{L}$ is minimised by η_2 and the order parameter jumps discontinuously from zero to η_1
- this is a first order phase transition
- note, that Landau theory is not strictly valid at such a transition, because the order parameter does not become arbitrarily small

Inhomogeneous systems

- to construct the Landau free energy, we assumed that a coarse graining procedure could be performed, which allowed to introduce a smoothly varying order parameter density
- so far, we have focussed on cases where this order parameter density is homogeneous in space
- the goal is to modify the Landau free energy such that it allows to describe inhomogeneous systems
- in order to see how to do this, we consider once more a magnetic system



here the system has a domain wall → this should cost energy

- it is energetically unfavourable to have large differences of magnetisation between adjacent blocks
- we need an extra term in the Landau free energy which penalises this
- this is for example achieved by a term that is proportional to the square of the gradient

$$\hookrightarrow \quad \left(m(x_n) - m(x_{n+1}) \right)^2 \sim \left(\nabla m(x) \right)^2$$

- using this choice, the Landau free energy becomes

$$L = \overbrace{\int d^d \vec{r}}^{\text{integration over } d\text{-dimension space}} \Big[\underbrace{\mathcal{L}(\{\eta(\vec{r})\})}_{\substack{\text{previously considered} \\ \text{Landau free energy density}}} + \frac{1}{2} \underbrace{\gamma}_{\substack{\text{positive} \\ \text{constant}}} \big(\underbrace{\nabla \eta(\vec{r})}_{\substack{\text{gradient of the} \\ \text{order parameter} \\ \text{density}}} \big)^2 \Big]$$

- note, that the choice of the „gradient term" has to be consistent with the symmetry, e.g. for the Ising magnet it should be invariant under $\eta(\vec{r}) \to -\eta(\vec{r})$
- for instance, we could have used as well a term of the type $\eta(\vec{r})\,\nabla^2\eta(\vec{r})$
- however, this is equivalent to $(\nabla\eta(r))^2$ due to $\nabla(\eta\nabla\eta) = \eta\nabla^2\eta + (\nabla\eta)^2$ and $\int d^d\vec{r}\;\nabla(\eta\nabla\eta) = \int d\vec{S}\cdot\eta\nabla\eta$ Gauss' theorem

$$\hookrightarrow \int d^d r\,\eta\nabla^2\eta = \underbrace{\int d\vec{S}\cdot\eta\nabla\eta}_{\substack{\text{surface}\\ \text{integral can}\\ \text{be neglected}\\ \text{in thermodynamic}\\ \text{limit}}} - \int d^d r\,(\nabla\eta)^2$$

$\hookrightarrow$ the choice $(\nabla\eta(\vec{r}))^2$ is the simplest and most general one that is compatible with the required symmetry

Correlation functions

- our goal is to obtain correlation functions from the partition function

$$Z = \mathop{\mathrm{Tr}}_{\eta(\vec{r})} e^{-\beta L(\{\eta(\vec{r})\})}$$

- this works pretty much the same way as for spins
- the difference is that the degrees of freedom $\eta(\vec{r})$ are labelled by the continuous variable $\vec{r}$, whereas the spins were labelled by a discrete index $i = 1, \dots, N$
- the current situation can be regarded as the continuum limit, in the sense that the lattice spacing $a \to 0$ and the number of degrees of freedom $N \to \infty$, such that the volume $V = N a^d$ remains constant

- let us now have a closer look at the formal aspects concerned with calculating the partition function
- the trace operation can be understood as the continuum limit of the functional integral

$$\mathrm{Tr} \equiv \int_{-\infty}^{\infty} \prod_{i=1}^{N} \underbrace{d\eta_i}_{\equiv d\eta(\vec{r}_i)} \quad , \text{ where } -\infty \leq \eta_i \leq \infty$$

- in practice functional integrals are often taken in <u>Fourier space</u>
- the corresponding transformation is defined as

$$\eta(\vec{r}) = \frac{1}{V} \sum_{\vec{k}} \hat{\eta}(\vec{k}) e^{i\vec{k}\cdot\vec{r}}$$

and $\hat{\eta}(\vec{k}) = \int_V d^d\vec{r}\; \eta(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}$

- we furthermore have $\frac{1}{V} \sum_{\vec{k}} e^{i\vec{k}(\vec{r}-\vec{r}')} = \delta(\vec{r}-\vec{r}')$

and in our calculations, we will often employ the replacement $\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^d} \int d^d\vec{k}$ when $V \to \infty$

- we also have, that

$$\int d^d\vec{r}\, e^{i(\vec{k}-\vec{k}')\vec{r}} = V \delta_{\vec{k}\vec{k}'} \quad \leftarrow \text{Kronecker-Delta}$$

in the $V \to \infty$ limit this expression becomes

$$\int d^d\vec{r}\, e^{i(\vec{k}-\vec{k}')\vec{r}} = (2\pi)^d\, \delta(\vec{k}-\vec{k}')$$

- usually, the order parameter densities $\eta(\vec{r})$ that we are dealing with are real
- this means that the Fourier components $\eta(\vec{k})$ and $\vec{\eta}(-\vec{k})$ are not idependent from one another, but are related via

$$\mathrm{Re}\, \hat{\eta}(\vec{k}) = \mathrm{Re}\, \hat{\eta}(-\vec{k}) \text{ and } \mathrm{Im}\, \hat{\eta}(\vec{k}) = -\mathrm{Im}\, \hat{\eta}(-\vec{k})$$

- (consequence of the fact that $\eta(\vec{r}) = \eta^*(\vec{r}) \to \eta(\vec{k}) = \eta^*(-\vec{k})$)
- this has to be taken into account when taking the trace in Fourier space (otherwise one would double count)

- an important tool for evaluating correlation functions is <u>functional differentiation</u>

- lets first illustrate the idea for a system with a finite number of degrees of freedom η_i, $i = 1, \dots, N$

- this system shall be described by a Hamiltonian $\mathcal{H}$ and a set of fields H_i, with couple linearly to the η_i

- the partition function then reads

$$Z = Z(\{H_i\}) = \mathrm{Tr}\, e^{-\beta(\mathcal{H} - \sum_i H_i \eta_i)}$$

and correlation functions can be calculated via differentiation

$$\langle \eta_i \eta_j \rangle = \frac{1}{\beta^2 Z(\{H_k\})} \frac{\partial}{\partial H_i} \frac{\partial}{\partial H_j} Z(\{H_k\})$$

- in the limit of infinitely many degrees of freedom the partition function becomes the so-called <u>generating functional</u>

$$Z(\{H(\vec{r})\}) = \mathrm{Tr}\, e^{-\beta\left[\mathcal{H} - \int d^d\vec{r}\, H(\vec{r})\, \eta(\vec{r})\right]}$$

- the partial derivatives have to be replaced by functional derivatives
- the functional derivative of a functional F with respect to $\eta(\vec{r})$ is defined as

$$\int d^d\vec{r}\, \frac{\delta F}{\delta \eta(\vec{r})}\, \phi(\vec{r}) = \lim_{\varepsilon\to 0} \frac{F[\eta(\vec{r})+\varepsilon\phi(\vec{r})] - F[\eta(\vec{r})]}{\varepsilon}$$

$$= \left[\frac{d}{d\varepsilon} F[\eta(\vec{r})+\varepsilon\phi(\vec{r})]\right]_{\varepsilon=0}$$

test function / „direction" into which the derivative is taken

c.f. vector calculus: derivative into direction of unit vector $\vec{n}$

$$(\nabla F)\cdot\vec{n} = \sum_j \frac{\partial F}{\partial x_j} n_j$$

$$= \lim_{\varepsilon\to 0} \frac{F[\vec{x}+\varepsilon\vec{n}] - F[\vec{x}]}{\varepsilon}$$

• Suppose now, that the functional is of the form $F[\eta(\vec r)] = \int d^d\vec r\, f(\vec r, \eta(\vec r), \nabla\eta(\vec r))$, then:

$$\int d^d\vec r \frac{\delta F}{\delta\eta(\vec r)}\phi(\vec r) = \left[\frac{d}{d\varepsilon}\int d^d\vec r\, f(\vec r, \eta(\vec r)+\varepsilon\phi(\vec r), \nabla\eta(\vec r)+\varepsilon\nabla\phi(\vec r))\right]_{\varepsilon=0}$$

$$= \int d^d\vec r\left[\frac{\partial f}{\partial\eta(\vec r)}\phi(\vec r) + \frac{\partial f}{\partial(\nabla\eta(\vec r))}\cdot\nabla\phi(\vec r)\right]$$

here we use the vector calculus identity
$\nabla\cdot(\psi\vec A) = \psi\nabla\cdot\vec A + \vec A\cdot\nabla\psi$

$$= \int d^d\vec r\left[\frac{\partial f}{\partial\eta(\vec r)}\phi(\vec r) + \nabla\cdot\left(\frac{\partial f}{\partial(\nabla\eta(\vec r))}\phi(\vec r)\right) - \left(\nabla\cdot\frac{\partial f}{\partial(\nabla\eta(\vec r))}\right)\phi(\vec r)\right]$$

can be converted into surface term that vanishes since $\phi(\pm\infty)=0$

$$= \int d^d\vec r\left[\frac{\partial f}{\partial\eta(\vec r)} - \nabla\cdot\frac{\partial f}{\partial(\nabla\eta(\vec r))}\right]\phi(\vec r)$$

- Since the latter expression holds for all $\phi(\vec r)$, we find that

$$\frac{\delta F}{\delta\eta(\vec r)} = \frac{\partial f}{\partial\eta(\vec r)} - \nabla\cdot\frac{\partial f}{\partial(\nabla\eta(\vec r))}$$

↳ $\frac{\delta}{\delta\eta(\vec r)}\int d^d\vec r\,'\,\eta(\vec r\,') = 1$; $\frac{\delta}{\delta\eta(\vec r\,')}\eta(\vec r) = \delta(\vec r - \vec r\,')$

$$\frac{\delta}{\delta\eta(\vec r)}\int d^d\vec r\,'\,\frac{1}{2}(\nabla\eta(\vec r\,'))^2 = -\nabla^2\eta(\vec r)$$

- before proceeding with the actual calculation of the correlation function, let us make some general statements first

- given a free energy $F(\{H(\vec{r})\})$, we can generate the expectation value of the order parameter

$$\langle \eta(\vec{r}) \rangle = -\frac{\delta F}{\delta H(\vec{r})}$$

and the generalised isothermal susceptibility

$$\chi_T(\vec{r}, \vec{r}\,') = \frac{\delta \langle \eta(\vec{r}) \rangle}{\delta H(\vec{r}\,')}$$

- for the latter one finds (following the calculation that we previously did for Ising systems):

$$\chi_T(\vec{r}, \vec{r}\,') = -\frac{\delta F}{\delta H(\vec{r})\,\delta H(\vec{r}\,')} = k_B T \left\{ \frac{1}{Z} \frac{\delta^2 Z}{\delta H(\vec{r})\,\delta H(\vec{r}\,')} - \frac{1}{Z}\frac{\delta Z}{\delta H(\vec{r})} \frac{1}{Z}\frac{\delta Z}{\delta H(\vec{r}\,')} \right\}$$

$$= \frac{1}{k_B T} \underbrace{\left\{ \langle \eta(\vec{r})\,\eta(\vec{r}\,') \rangle - \langle \eta(\vec{r}) \rangle \langle \eta(\vec{r}\,') \rangle \right\}}_{\substack{\text{connected correlation} \\ \text{function } G(\vec{r}, \vec{r}\,'), \\ \text{two-point correlation function}}}$$

- for translationally invariant systems, we have $\chi(\vec{r},\vec{r}\,') = \chi(\vec{r}-\vec{r}\,')$ and $G(\vec{r},\vec{r}\,') = G(\vec{r}-\vec{r}\,')$
- this yields the principal result of

<u>linear response theory</u>

correlation function "response function"

$$G(\vec{r}-\vec{r}\,') = k_B T \, \chi_T(\vec{r}-\vec{r}\,')$$

response of the order parameter to external perturbations

$$\delta \langle \eta(\vec{r}) \rangle = \int d^d r' \, \chi_T(\vec{r}-\vec{r}\,') \, \delta H(\vec{r}\,')$$

- in Fourier space this relation reads

$$\hat{\chi}_T(\vec{k}) = \beta \, \hat{G}(\vec{k})$$

- from this expression we can derive the sum rule

$$\chi_T \equiv \lim_{\vec{k}\to 0} \hat{\chi}_T(\vec{k}) = \beta \, \hat{G}(\vec{k})\Big|_{\vec{k}=0} = \beta \int d^d r \, G(\vec{r})$$

- we found this relation actually already, when we studied the Ising model

- we now calculate the two-point correlation function
- to do so, we first take the functional derivative of the Landau free energy with respect to $\eta(\vec{r})$ and demand stationarity:

$$\frac{\delta L}{\delta \eta(\vec{r})} = \frac{\delta}{\delta \eta(\vec{r})} \int d^d r' \left[\frac{\gamma}{2} (\nabla \eta(\vec{r}'))^2 + a t \eta^2(\vec{r}') + \frac{1}{2} b \eta^4(\vec{r}') - H(\vec{r}')\eta(\vec{r}') \right]$$

$$= -\gamma \nabla^2 \eta(\vec{r}) + 2at\,\eta(\vec{r}) + 2b\,\eta^3(\vec{r}) - H(\vec{r})$$

$$\stackrel{!}{=} 0$$

- in the next step, we perform the derivative with respect to the external field $H(\vec{r}')$

$$\frac{\delta}{\delta H(\vec{r}')} \left(-\gamma \nabla^2 \eta(\vec{r}) + 2at\,\eta(\vec{r}) + 2b\,\eta^3(\vec{r}) - H(\vec{r}) \right)$$

$$= \left(-\gamma \nabla^2 + 2at + 6b\,\eta^2(\vec{r}) \right) \chi_T(\vec{r}-\vec{r}') - \delta(\vec{r}-\vec{r}') = 0$$

- expressing $\chi_T(\vec{r}-\vec{r}')$ through $G(\vec{r}-\vec{r}')$ yields

$$\beta \left(-\gamma \nabla^2 + 2at + 6b\,\eta^2(\vec{r}) \right) G(\vec{r}-\vec{r}') = \delta(\vec{r}-\vec{r}')$$

the two-point correlation function is actually a Green function!

- we now find in the symmetric ($t>0$) phase, where $\eta(\vec{r}) = \eta = 0$

$$\left(-\nabla^2 + \xi_>^{-2}\right) G(\vec{r}-\vec{r}\,') = \frac{k_B T}{\gamma} \delta(\vec{r}-\vec{r}\,') \; ; \; \xi_> = \sqrt{\frac{\gamma}{2at}}$$

- in the symmetry broken phase ($t<0$), we have insted

$$\left(-\nabla^2 + \xi_<^{-2}\right) G(\vec{r}-\vec{r}\,') = \frac{k_B T}{\gamma} \delta(\vec{r}-\vec{r}\,') \; ; \; \xi_< = \sqrt{-\frac{\gamma}{4at}}$$

- here $\xi_{\gtrless}$ represent the correlation length, which above and below the transition behaves as $\xi \propto \begin{cases} |t|^{-\nu}, & t>0 \\ |t|^{-\nu'}, & t<0 \end{cases}$ and hence we find the critical exponents $\nu = \nu' = 1/2$
- let us now find an explicit expression for the two-point correlation function
- first we consider how it behaves at the critical point, where $\xi \to \infty$
- introducing the Fourier transform and using that $\nabla^2 G(\vec{r}-\vec{r}\,') \to -|\vec{k}|^2 \hat{G}(\vec{k}) = -k^2 G(\vec{k})$, we find

$$\hat{G}(\vec{k}) = \frac{k_B T}{\gamma} \frac{1}{k^2 + \xi^{-2}} \xrightarrow{\xi \to \infty} \frac{1}{k^2}$$

- for $d > 2$ this yields

$$G(\vec{r}-\vec{r}\,') = G(|\vec{r}-\vec{r}\,'|) = G(r) \propto \frac{1}{r^{d-2}},$$

i.e. the correlations decay as a power law at the critical point

- we will now derive a more general expression
- to this end we return to the differential equation for $G(\vec{r}-\vec{r}\,')$, set $\vec{r}\,'=0$ and transform to d-dimensional spherical coordinates (assuming spatial isotropy)

$$\hookrightarrow \left[-\frac{1}{r^{d-1}}\frac{\partial}{\partial r} r^{d-1}\frac{\partial}{\partial r} + \xi^{-2}\right] G(r) = \frac{k_B T}{\gamma}\,\delta(r)$$

- introducing the scaled coordinate $\rho = \frac{r}{\xi}$ and using $\mathcal{G}(\rho) = G(\frac{r}{\xi})$ and $\delta(\rho\xi) = \frac{1}{\xi^d}\,\delta(\rho)$, one obtains

$$\left[-\frac{1}{\rho^{d-1}}\frac{\partial}{\partial \rho}\rho^{d-1}\frac{\partial}{\partial \rho} + 1\right]\mathcal{G}(\rho) = g\,\delta(r)$$

$$\uparrow$$

$$g = \frac{k_B T}{\gamma}\,\xi^{2-d}$$

- this differential equation can be solved in terms of the so-called modified spherical Bessel functions of the third kind, $K_n(\rho)$

$$\hookrightarrow \frac{1}{g}\,\mathcal{G}(\rho) = \begin{cases} \overbrace{e^{-\rho}}^{\text{exponentially decaying correlations in 1d}} & , d = 1 \\ \frac{1}{(2\pi)^{d/2}}\,\rho^{-\frac{d-2}{2}}\,K_{\frac{d-2}{2}}(\rho) & , d \geq 2 \end{cases}$$

- the Bessel functions have the following asymptotic properties:

$$K_n(\rho) \sim \left(\frac{\pi}{2\rho}\right)^{1/2} e^{-\rho} \qquad \text{for } \rho \to \infty$$

$$K_n(\rho) \sim \frac{\Gamma(n)}{2}\left(\frac{\rho}{2}\right)^{-n} \qquad \text{for } \rho \to 0$$
$$K_0(\rho) \sim -\operatorname{Log}(\rho)$$

- we thus obtain away from criticality, where $r \gg \xi$ ($\rho \gg 1$) and for $d \geq 2$

$$G(r) \propto \frac{k_B T}{\gamma}\,\frac{1}{\xi^{\frac{d-3}{2}}}\,\frac{e^{-r/\xi}}{r^{\frac{d-1}{2}}}$$

- at the critical point, on the other hand, ξ is diverging and hence with $r \ll \xi$ ($\xi \ll 1$) we obtain the known result

$$G(r) \sim \frac{k_B T}{\gamma} \frac{1}{r^{d-2}} \qquad \text{for } d > 2$$

- additional remarks:

- from $\hat{G}(\vec{k}) = \frac{k_B T}{\gamma} \frac{1}{k^2 + \xi^{-2}}$, we find by using the sum rule $\chi_T = \beta \hat{G}(0)$, that $\chi_T = \frac{\xi^2}{\gamma}$
- given, that $\xi \sim t^{-1/2}$, one finds a critical exponent: $\chi_T \sim |t|^{-\gamma} \rightarrow \gamma = 1$
- experimentally, one finds that the two-point correlations at criticality behave as $G(r) \propto \frac{1}{r^{d-2+\eta}}$, where η is another critical exponent (predicted to be zero by Landau theory)
- η is linked to the so-called anomalous dimension

Fluctuations and breakdown of Landau theory

- Landau theory is in spirit some kind of mean field theory in the sense that it assumes that fluctuations are small and that the physics of the system of interest can be described by a smoothly varying order parameter (density)
- the length scale with respect to which the smoothly varying order parameter is defined is of the order of the correlation length ξ
- the comparision between the fluctuations and the typical magnitude of the order parameter on the range of this length scale can be undertaken by studying the ratio

$$E_{LG} = \frac{\left| \int_V d^d\vec{r}\, G(\vec{r}) \right|}{\int_V d^d\vec{r}\, \eta^2(\vec{r})}$$

with the integration value $V = \xi^d$

- when E_{LG} is small Landau theory should be applicable
- this is referred to as <u>the Ginzburg criterion</u>

- using the Landau free energy of the Ising model, we can estimate the denominator of E_{LG} using

$$\int_V d^d\vec{r}\,\eta^2(\vec{r}) \approx \underset{\uparrow}{\xi^d} \cdot \underbrace{\frac{a}{b}|t|}_{\substack{\text{value of } \eta^2 \\ \text{in symmetry} \\ \text{broken phase}}} = \xi_0^d \frac{a}{b} |t|^{1-\frac{d}{2}}$$

$$\xi = \xi_0 |t|^{-1/2}$$

- for the numerator we estimate

$$\int_V d^d\vec{r}\, G(\vec{r}) \approx k_B T_c \chi_T \propto \frac{k_B T_c}{a|t|}$$

- this yields

$$E_{LG} = \frac{k_B T_c}{a|t|} \cdot \frac{b}{a\xi_0^d |t|^{1-\frac{d}{2}}} = \frac{k_B}{\Delta C \xi_0^d} \frac{1}{|t|^{2-\frac{d}{2}}},$$

where we have introduced $\Delta C = \frac{a^2}{b} T_c$, which is the jump in heat capacity at the phase transition

- requiring that $E_{LG} \ll 1$ thus leads to

$$|t|^{\frac{4-d}{2}} \gg \frac{k_B}{\Delta C \, \xi_0^d} \equiv t_{LG}^{\frac{4-d}{2}}$$

value of the temperature that marks onset of critical region (fluctuations become very large)

- apparently, the applicability of Landau theory depends on dimensionality

$d>4$: as $t \to 0$ the Ginzberg criterion is always satisfied

$d<4$: the Ginzberg criterion is not satisfied and the „correct" physics is not described by Landau theory

$d=4$: Landau theory is not quite correct, but acquires corrections from fluctuations, eg one finds

$$\chi_T \sim \frac{1}{t} |\log t|^{1/3}$$

logarithmic correction

- so far we have focused the discussion on the Landau free energy related to the Ising universality class
- Similar considerations can be made for other models, and one finds that the dimension above which Landau theory becomes exact may change
- quite generally one finds

$$\int_V d^d\vec{r}\, G(\vec{r}) \sim k_B T \chi_T \sim t^{-\gamma}$$

$$\int_V d^d\vec{r}\, \eta^2(\vec{r}) \sim \xi^d |H|^{2\beta} \sim t^{2\beta-\nu d},$$

and requiring $E_{LG} \ll 1$ leads to

$$t^{-\gamma} \ll t^{2\beta-\nu d} \quad \text{as } t \to 0$$

- this is true, when

$$d > \frac{2\beta+\gamma}{\nu} \equiv d_c$$

<u>upper critical dimension</u>

- next, we discuss how fluctuations around the homogeneous order parameter density can affect thermodynamic quantities
- to this end we study the so-called

Gaussian model

- let us consider a Hamiltonian that depends on the variables $\vec{q} = (q_1, \dots, q_N)$
- this Hamiltonian shall assume a minimum at $\vec{q} = \vec{q}_0 = (q_1^0, \dots, q_N^0)$
- Taylor expanding around this minimum yields

$$\mathcal{H}(\vec{q}) \approx \mathcal{H}(\vec{q}_0) + \frac{1}{2} \sum_{\alpha,\beta=1}^{N} (q_\alpha - q_\alpha^0) \left.\frac{\partial^2 \mathcal{H}(\vec{q})}{\partial q_\alpha \partial q_\beta}\right|_{\vec{q}=\vec{q}_0} (q_\beta - q_\beta^0) + \dots$$

- the matrix $M_{\alpha\beta} = \left.\frac{\partial^2 \mathcal{H}(\vec{q})}{\partial q_\alpha \partial q_\beta}\right|_{\vec{q}=\vec{q}_0}$ is the so-called fluctuation matrix
- diagonalising this matrix yields the normal modes $\vec{v}^{(i)}$

$$\sum_\beta M_{\alpha\beta} v_\beta^{(i)} = \tilde{\lambda}_i v_\alpha^{(i)}$$

$\uparrow$ eigenvalues

$\hookrightarrow$ normal coordinates

$$q_i' = \sum_{\alpha=1}^{N} v_\alpha^{(i)} (q_\alpha - q_0)$$

- reparameterising $\frac{1}{\lambda_i^2} = \beta \tilde{\lambda}_i$, we can write the Hamiltonian:

$$\beta \mathcal{H}(\vec{q}) \approx \beta \mathcal{H}(\vec{q}_0) + \frac{1}{2} \sum_{\alpha=1}^{N} \frac{(q_\alpha')^2}{\lambda_\alpha^2}$$

- we can now write for the partition function $Z = e^{-\beta G}$

$$e^{-\beta G} = \int_{-\infty}^{\infty} \prod_{i=1}^{N} dq_i \, e^{-\beta \mathcal{H}(\vec{q})}$$

$$\approx e^{-\beta \mathcal{H}(\vec{q}_0)} \int_{-\infty}^{\infty} \prod_{i=1} dq_i \, e^{-\frac{\beta}{2} \sum_{\alpha\beta} (q_\alpha - q_\alpha^0) M_{\alpha\beta} (q_\beta - q_\beta^0)}$$

$$= e^{-\beta \mathcal{H}(\vec{q}_0)} \int_{-\infty}^{\infty} \prod_{i=1} dq_i' \, e^{-\frac{1}{2} \sum_\alpha \frac{(q_\alpha')^2}{\lambda_\alpha^2}}$$

$$= e^{-\beta \mathcal{H}(\vec{q}_0)} \prod_{i=1} \underbrace{\int_{-\infty}^{\infty} dq_i' \, e^{-\frac{1}{2} \frac{(q_i')^2}{\lambda_i^2}}}_{\text{Gaussian integral } = \sqrt{2\pi}\,\lambda_i}$$

$\hookrightarrow \quad G = \mathcal{H}(\vec{q}_0) - \frac{1}{2} k_B T \sum_{i=1}^{N} \log (2\pi \lambda_i^2)$

- we will apply this methodology now for calculating $Z = \mathrm{Tr}_{\eta(\vec{r})}\, e^{-\beta L(\{\eta(\vec{r})\})}$ with the Landau free energy

$$L = \int d^d\vec{r} \left[\frac{1}{2}\gamma (\nabla \eta(\vec{r}))^2 + a t\, \eta^2(\vec{r}) \right] \text{(+ constant)}$$

- this L is obtained by neglecting the $\eta^4(\vec{r})$ in the Ising model Landau free energy (for $T > T_c$), but can also be obtained by expanding around $\eta = \pm\sqrt{-\frac{a}{b}t}$ in the symmetry broken phase

- the first step is to go to Fourier space:

$$L = \int d^d\vec{r} \left[\frac{\gamma}{2} (\nabla \eta(\vec{r}))^2 + a t\, \eta^2(\vec{r}) \right]$$

$$= \frac{1}{V^2} \sum_{\vec{k}\vec{k}'} \int d^d\vec{r} \left[\frac{\gamma}{2} (i)^2\, \vec{k}\cdot\vec{k}' + a t \right] \hat{\eta}(\vec{k})\, \hat{\eta}(\vec{k}')\, e^{i(\vec{k}+\vec{k}')\cdot\vec{r}}$$

$$= \frac{1}{V} \sum_{\vec{k},\vec{k}'} \left[\frac{\gamma}{2} (-\vec{k}\cdot\vec{k}') + a t \right] \hat{\eta}(\vec{k})\, \hat{\eta}(\vec{k}')\, \delta_{\vec{k},-\vec{k}'}$$

$$= \frac{1}{V} \sum_{\vec{k}} \frac{1}{2} \left[\gamma k^2 + 2 a t \right] |\hat{\eta}(\vec{k})|^2$$

$$\rightarrow \quad Z = \int_{-\infty}^{\infty} \prod_{\vec{k}}{}' \, d\hat{\eta}(\vec{k}) \, e^{-\beta L}$$

↑ only momenta with $|\vec{k}| \geq 0$ (see „double counting" on page 22)

$$= \prod_{\vec{k}}{}' \int_{-\infty}^{\infty} d\hat{\eta}(\vec{k}) \, e^{-\frac{\beta}{2V}(\gamma k^2 + 2at)|\hat{\eta}(\vec{k})|^2}$$

$$= \prod_{\vec{k}}{}' \int_{-\infty}^{\infty} d\,\mathrm{Re}(\hat{\eta}(\vec{k}))\, d\,\mathrm{Im}(\hat{\eta}(\vec{k}))\, e^{-\frac{\beta}{2V}(\gamma k^2 + 2at)\left[(\mathrm{Re}\,\hat{\eta}(\vec{k}))^2 + (\mathrm{Im}\,\hat{\eta}(\vec{k}))^2\right]}$$

- using $\int_{-\infty}^{\infty} dx\,dy\, e^{-A(x^2+y^2)} = \frac{\pi}{A}$

factor emerges because we sum over the whole k-space

$$e^{-\beta\Delta G} = \prod_{\vec{k}}{}' \frac{2\pi V k_B T}{2at + \gamma k^2} = \exp\left\{ \frac{1}{2} \sum_{|\vec{k}|<\Lambda} \log\left[\frac{2\pi V k_B T}{2at + \gamma k^2}\right] \right\}$$

change of free energy due to fluctuations

cut-off momentum scale, e.g. given by lattice spacing

↳ apparently fluctuations change the free energy:

$$G = G_0 + \Delta G = G_0 - \frac{1}{2} k_B T \sum_{|\vec{k}|<\Lambda} \log\left[\frac{2\pi V k_B T}{2at + \gamma k^2}\right]$$

- we can now calculate how this change to the free energy affects the heat capacity; $C_V = -T \frac{\partial^2 G}{\partial T^2}$

$$\hookrightarrow \frac{C_V}{TV} = \frac{c_V}{T} = \frac{1}{2}\frac{\partial^2}{\partial T^2}\frac{k_B T}{V}\sum_{|\vec{k}|<\Lambda} \log\left[\frac{2\pi V}{2at+\gamma k^2}\right] + \underbrace{\frac{1}{2V}\frac{\partial^2}{\partial T^2}k_B T \log(k_B T)\cdot \sum_{|\vec{k}|<\Lambda} 1}_{=\frac{k_B}{2VT}\sum_{|\vec{k}|<\Lambda} 1}$$

(temperature independent contrib. to C_V neglected in the following)

- taking the derivatives and converting the sum into an integral, results in

last term in above equation neglected

$$\frac{c_V}{T} = \frac{2a^2 k_B T}{T_c^2}\underbrace{\int_{|\vec{k}|<\Lambda}\frac{d^d\vec{k}}{(2\pi)^d}\frac{1}{(2at+\gamma k^2)^2}}_{I_1} - \frac{2a k_B}{T_c}\underbrace{\int_{|\vec{k}|<\Lambda}\frac{d^d\vec{k}}{(2\pi)^d}\frac{1}{2at+\gamma k^2}}_{I_2}$$

- to calculate the critical exponent α, which is associated with the behaviour of the heat capacity near the critical point, we now study how the two integrals behave when approaching $t\to 0^+$, where $\xi \to 0$
- introducing $\xi^{-2} = \frac{2a}{\gamma}t$, we write

$$I_1 = \frac{1}{\gamma^2}\int_{|\vec{k}|<\Lambda}\frac{d^d\vec{k}}{(2\pi)^d}\frac{1}{(\xi^{-2}+k^2)^2} \overset{\vec{q}=\xi\vec{k}}{=} \xi^{4-d}\frac{1}{\gamma^2}\int_{|\vec{k}|<\xi\Lambda}\frac{d^d\vec{q}}{(2\pi)^d}\frac{1}{(1+q^2)^2}$$

- the integral

$$\int_{|\vec{k}|<\xi\Lambda} d^d\vec{q}\, \frac{1}{(1+q^2)^2} \overset{\xi\to\infty}{\propto} \int_0^\infty dq\, \frac{q^{d-1}}{(1+q^2)^2}$$

converges for $d<4$ and hence $I_1 \propto \xi^{(4-d)}$

- for $d>4$ one finds that I_1 approaches a constant, since $I_1 \sim \int_0^\Lambda dk\, k^{d-1-4} = \text{const.}$
- in summary: $I_1 \propto \begin{cases} \xi^{(4-d)} \propto t^{-(2-\frac{d}{2})} & ; d<4 \\ \text{finite (no divergence)} & ; d>4 \end{cases}$

- for the integral I_2 a similar analysis shows, that $I_2 \sim \xi^{(2-d)} \sim t^{-(1-\frac{d}{2})}$ for $d<2$ and that I_2 is finite for $d>2$

↳ the dominant divergence stems from I_1

- for the heat capacity we thus obtain the scaling

$$c_V \sim \begin{cases} t^{-\alpha} & ; d<4 \\ \text{finite} & ; d>4 \end{cases}$$

where $\alpha = 2-\frac{d}{2}$

- this is different to the mean field result, which was $\alpha=0$ and therefore fluctuations may indeed change critical exponents

Critical exponents and scaling hypothesis

- Landau theory successfully describes the qualitative behaviours of matter near phase transitions
- however, many quantitative aspects, which are observed in experiment are not quantitatively captured, e.g. the values of the critical exponents and their dependence on dimensionality
- a better description of critical phenomena can be made by introducing the so-called scaling hypothesis which is motivated by the observation that the universality of critical phenomena is due to the scale invariance of thermodynamic quantities near the critical point

- let us begin by gathering the critical exponents:

α ... scaling of the heat capacity: $C_V \sim |t|^{-\alpha}$

β ... scaling of the order parameter: $\eta \sim |t|^{\beta}$

γ ... scaling of the susceptibility: $\chi_T \sim |t|^{-\gamma}$

δ ... scaling of the order parameter with respect to conjugate field: $\eta \sim H^{1/\delta}$

ν ... scaling of the correlation length: $\xi \sim |t|^{-\nu}$

η ... scaling of the correlation function: $G(r) \sim \frac{1}{r^{d-2+\eta}}$

↑ not to be confused with order parameter

- in fact not all of these exponents are independent and relations among them are established via the so-called <u>scaling relations / laws</u>

- these relation are derived be assuming that the free energy density, which has the unit of inverse volume, scales at the critical point (phase transition point) as $f \sim \xi^{-d} \sim |t|^{d\nu}$

- this means that at the critical point the correlation length ξ is considered to be the only relevant length scale
- under this assumption, we can derive the first relation between critical exponents by calculating the heat capacity

$$c_V = -T_c \frac{\partial^2 f}{\partial T^2} = -\frac{1}{T_c}\frac{\partial^2 f}{\partial t^2} \sim \frac{|t|^{d\nu}}{t^2} \sim |t|^{d\nu-2}$$

- this yields the <u>Josephson scaling law</u>

$$d\nu = 2-\alpha$$

- the second relation is obtained from the correlation function
- introducing the scaled length $\rho = r/\xi$ one finds that the physical scale of

$$G(r) = G(\xi\rho) \sim \xi^{-d+2-\eta}\frac{1}{\rho^{d-2+\eta}} = \xi^{-d+2-\eta}\,\underset{\substack{\uparrow \\ \text{dimensionless} \\ \text{"scaling function"}}}{G(\rho)}$$

$$\xi^{-d+2-\eta} \sim |t|^{\nu(d-2+\eta)}$$

- on the other hand $G(r) \sim \eta^2 \sim |t|^{2\beta}$, which yields $2\beta = \nu(d-2+\eta)$

- the third relation is obtained from susceptibility sum rule $\chi_T = \beta \int d^d\vec{r}\, G(\vec{r})$
  ↳ $\chi_T \sim \xi^d \xi^{-d+2-\eta} = \xi^{2-\eta} \sim |t|^{-\nu(2-\eta)}$
- this yields the <u>Fisher scaling law</u>

$$\gamma = \nu(2-\eta)$$

- the final relation we obtain from $\eta = -\frac{\partial f}{\partial H}\Big|_{H=0}$
- since $f \sim \xi^{-d}$ and $\eta \sim |t|^\beta \sim \xi^{-\frac{\beta}{\nu}} = \xi^{-\frac{1}{2}(d-2+\eta)}$, it must be the case that $H \sim \xi^{\frac{1}{2}(-d-2+\eta)}$
  $\sim |t|^{\nu/2(d+2-\eta)}$
- on the other hand we have $\eta \sim H^{1/\delta}$ and thus $H \sim \eta^\delta \sim |t|^{\beta\delta}$
- this yields $\beta\delta = \frac{\nu}{2}(d+2-\eta)$, and by subtracting $\beta = \frac{\nu}{2}(d-2+\eta)$ we obtain $\beta(\delta-1) = \nu(2-\eta) = \gamma$, which is the so-called <u>Widom scaling law</u>
- finally, by adding $\beta\delta = \frac{\nu}{2}(d+2-\eta)$ and $\beta = \frac{\nu}{2}(d-2+\eta)$, and using the Widom scaling law, one obtains the <u>Rushbrooke scaling law</u>: $\alpha + 2\beta + \gamma = 2$

- the six critical exponents obey 4 scaling laws, which shows that only two exponents are actually independent and sufficient to describe critical behaviour near a continuous phase transition

Phenomenological scaling theory

- the scaling laws were derived on the basis that near a continuous phase transition the correlation length ξ dominates over all other length scales
- we will now discuss an elegant way to formalise this scaling behaviour
- this is based on the observation that when all observables exhibit scaling behaviour near the critical point, they must be homogeneous functions of some scaling parameters λ_i, which all are eventually related to the correlation length $\xi \sim |t|^{\nu}$

- a homogeneous function satisfies
$$g(x) = b^a g(bx)$$
(for example: $g(x) = ax^c$; $g(bx) = b^c a x^c \rightarrow g(x) = b^{-c} g(bx)$)

- at the critical point the correlation function $G(r)$ is homogeneous: $G(r) = b^{-(d-2+\eta)}\, G(b^{-1} r)$
- this means that the correlation function at a distance r is the same as the correlation function at the smaller distance $b^{-1} r$ (assuming $b > 1$), when the latter is multiplied by $b^{-(d-2+\eta)}$
- hence, the form of $G(r)$ is invariant under the scale transformation $r \rightarrow b^{-1} r$
- this is referred to as <u>scale invariance</u>

- when moving away from the critical point, the distance scale is set by the correlation length $\xi \sim t^{-\nu}$
- the scaling hypothesis is the assumption that the correlation function away (but close to) from the critical point is invariant under a rescaling of the length scales by the correlation length

- away from the critical point, the correlation function depends on distance and temperature, leading to the scaling form

$$G(r,t) = b^{-(d-2+\eta)}\, G(b^{-1} r,\, b^{1/\nu} t)$$

in order to get the the correct dimension, assuming that b is a length

- we now choose $b = t^{-\nu}$, which means that we indeed rescale all lengths proportionally to the correlation length
- this leads to $G(r,t) = t^{\nu(d-2+\eta)}\, G(t^{\nu} r)$, i.e. the correlation function depends only on the combination $t^{\nu} r$
- using now that $\chi_T \sim \int d^d r\, G(r,t)$ and $\chi_T \sim |t|^{-\gamma}$, this leads immediately to the Fisher scaling law: $\gamma = \nu(2-\eta)$
- a scaling form can also be derived for thermodynamic functions, such as the free energy density, which depends on t and the magnetic field H:

$$f(t,H) = t^{2-\alpha}\, f(|t|^{-\beta\delta} H)$$

- from this follows for the magnetisation density

$$\eta \sim \frac{\partial}{\partial H} f(t,H) \sim t^{2-\alpha-\beta\delta} M(|t|^{-\beta\delta} H)$$

- with $\eta \sim t^{\beta}$ we find that $\beta = 2-\alpha-\beta\delta$, which is consistent with the previously found scaling relations

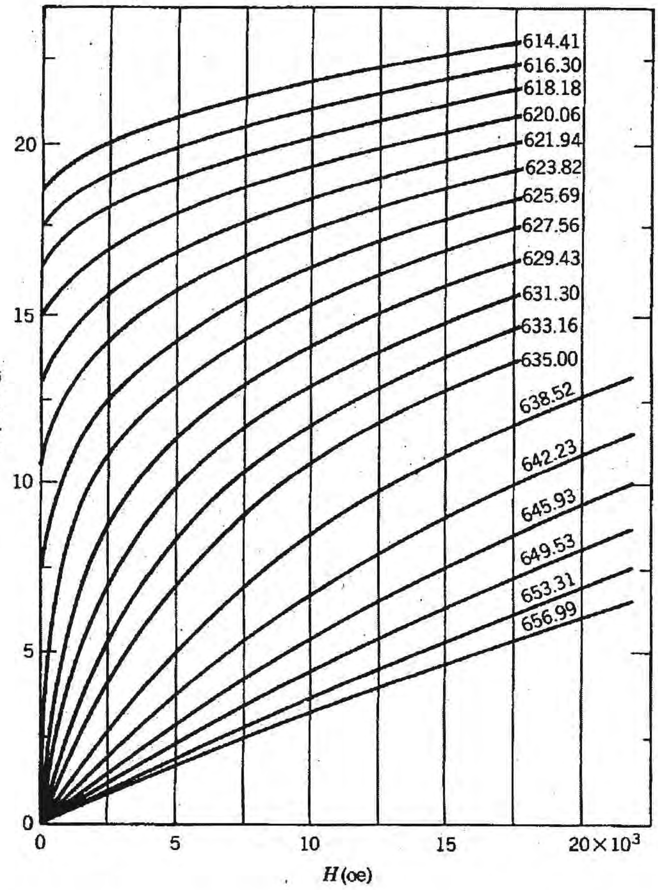
- hence $\eta \sim t^{\beta} \underbrace{S(|t|^{-\beta\delta} H)}_{\text{scaling function}}$

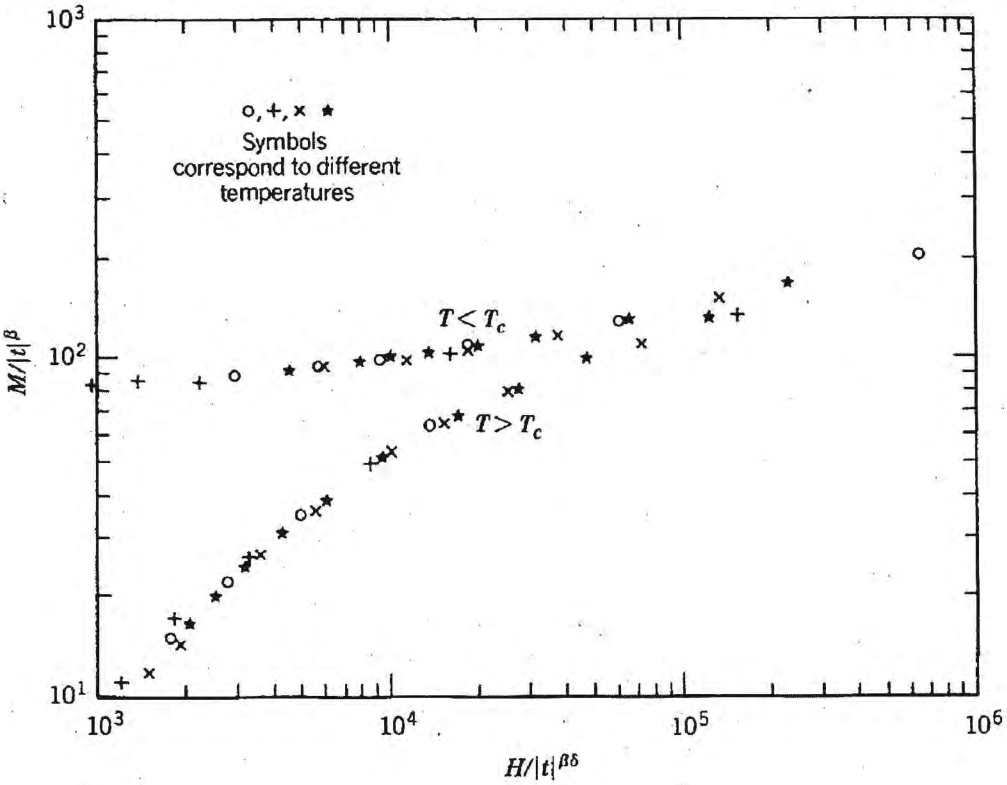
- this expression shows that the magnetisation density follows a universal behaviour near the phase transition point
- the scaling function S is typically different below and above T_c
- this result implies that when plotting $\eta |t|^{-\beta}$ as a function of $|t|^{-\beta\delta} H$ the results should collapse on a universal curve
- this is indeed observed for experimental data

Magnetisation of nickel
Weiss and Forrer (1926)

$T_c = 627.2$ K
$\beta = 0.368$
$\delta = 4.22$

for the 3d Ising model one would expect $\beta = 0.326$ and $\delta = 4.790$





Kerson Huang
Statistical Physics
John Wiley and Sons (1987)

Anomalous dimension

- to conclude the discussion of the Landau free energy we perform a dimensional analysis
- the partition function is given by

$$Z = \int D\eta \, \exp\left\{-\beta \int d^d\vec{r} \left[\frac{\gamma}{2}(\nabla\eta)^2 + at\eta^2 + \frac{1}{2}b\eta^4\right]\right\}$$

- the exponent has to have dimension 1, i.e. it scales as l^0, where l is the unit of length
- assuming that $[\beta\gamma] = l^0$, one has

$$\left[\int d^d\vec{r}\, (\nabla\eta)^2\right] = \underbrace{\left[\int d^d\vec{r}\right]}_{l^d} \cdot \Big(\underbrace{[\nabla]}_{l^{-1}} \cdot \underbrace{[\eta]}_{l^{d_\eta}}\Big)^2 \overset{!}{=} l^0$$

$\leftarrow$ dimension of η

$\hookrightarrow d - 2(1 - d_\eta) = 0$

- from this follows that the dimension of η is given by $d_\eta = -\frac{d-2}{2}$ (= "canonical" dimension)
- this sets in principle also the dimension of other quantities, obtained from η

- for example, one would expect, that the dimension of the correlation function $G(\vec{r},\vec{r}') = \frac{1}{k_B T}\{\langle\eta(\vec{r})\eta(\vec{r}')\rangle - \langle\eta(\vec{r})\rangle\langle\eta(\vec{r}')\rangle\}$ is given by $2d_\eta$, i.e. $[G(\vec{r},\vec{r}')] = \ell^{-d+2}$
- however, in actual experiments one finds $[G(\vec{r},\vec{r}')] = \ell^{-d+2+\eta}$
- apparently, this scaling is contradicting the dimensional analysis, which is the reason why η is referred to as anomalous dimension
- the reason for its appearance is that the averaging, $\langle\cdot\rangle$, introduces another length scale, e.g., associated with lattice spacing a or the momentum (wave number) cut-off $\Lambda \sim \frac{1}{a}$
- so, strangely, close to the phase transition there is another length scale, besides ξ, which controls the physics

- this has to be accounted for in the scaling function, and instead of

$$\eta(x/b) = b^{d_\eta}\,\eta(x) \quad \text{with } d_\eta = \frac{d-2}{2}$$

one has

$$\langle \eta(x/b, a/b) \rangle = b^{D} \langle \eta(x, a) \rangle \quad \text{with}$$

$$D = d_\eta + \frac{\eta}{2}$$

Renormalisation group

- the basic idea behind the renormalisation group can be illustrated by studying a ferromagnet and introducing the concept of <u>block spins</u>

- the Hamiltonian of N spins on a d-dimensional hypercubic lattice is given by

$$\beta \mathcal{H} = -\underbrace{\beta J}_{K} \sum_{\langle ij \rangle}^{N} S_i S_j - \underbrace{\beta H}_{h} \sum_{i}^{N} S_i$$

- near the phase transition at T_c spins are correlated on lengths of the order of $\xi(T)$

- therefore, there are blocks of spins of size $la \ll \xi(T)$, where a is the lattice spacing, that effectively act like a single spin = block spin

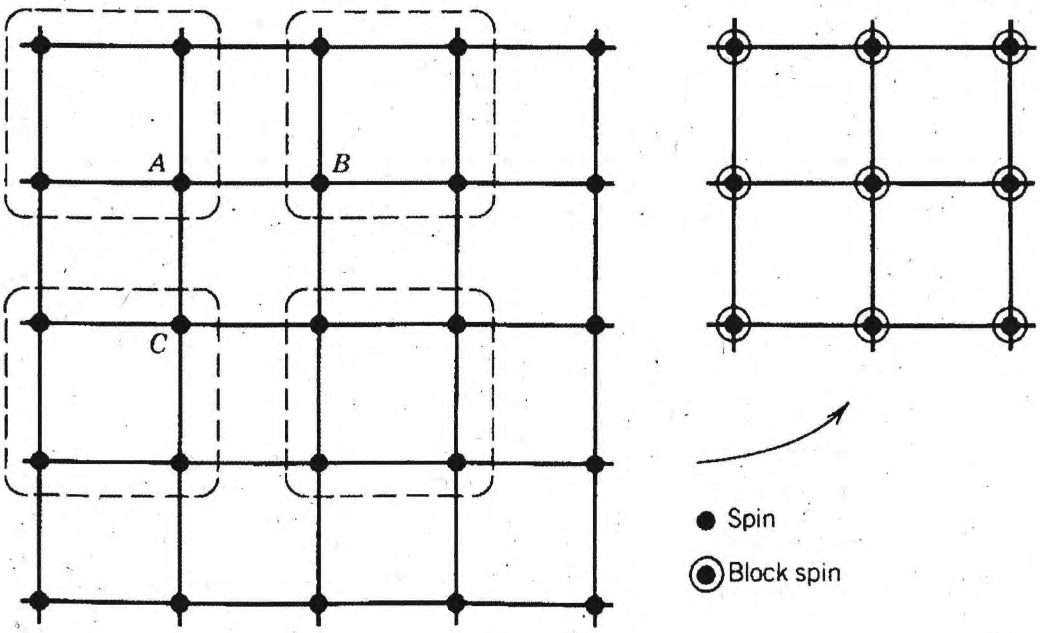


Fig. 18.1 Block-spin transformation: averaging the spins in a block, and then rescaling the lattice to the original size. In more than one dimension, the indirect interaction between B and C gives rise to next-to-nearest-neighbor interactions of the block spins.

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- each block spin contains ℓ^d spins, and hence the number of block spins is $\ell^{-d} N$

- the block spins are formally defined as

$$S_I = \frac{1}{|\overline{m}_\ell|} \frac{1}{\ell^d} \sum_{i \in I} s_i \quad , \text{ where}$$

label of a block $\nearrow$ (I)

$$\overline{m}_\ell = \frac{1}{\ell^d} \sum_{i \in I} s_i \quad \text{is the average}$$

magnetisation of the block I

- with this definition the range of values that a block spin can take is identical to that of the individual spins: $S_I = \begin{cases} +1 \\ -1 \end{cases}$

- the assumption is now (pioneered by Kadanoff), that the Hamiltonian expressed in terms of the block spins has the same form as the initial Hamiltonian, but with different coupling constants K_ℓ and h_ℓ (for $\ell = 1$ we have the original couplings: $K_1 = K$; $h_1 = h$)

$$\hookrightarrow \beta \mathcal{H}_\ell = -K_\ell \sum_{\langle IJ \rangle}^{N\ell^{-d}} S_I S_J - h_\ell \sum_{I=1}^{N\ell^{-d}} S_I$$

- there are fewer block spins than original spins, and therefore the correlation length ξ_ℓ, which is measured in units of ℓa is smaller than the correlation length ξ_1 of the initial system
  $\hookrightarrow$ $\xi_\ell = \dfrac{\xi_1}{\ell}$
- thus, since $\xi_\ell < \xi_1$, the Hamiltonian $\mathcal{H}_\ell$ is further away from criticality than the original one
  $\hookrightarrow$ so the effective temperature t_ℓ must have increased
- similarly, the magnetic field is rescaled according to $h \sum_i s_i \simeq h \bar{m}_\ell \ell^d \sum_I S_I \equiv h_\ell \sum_I S_I$
- given that the original and the new Hamiltonian are of the same form, also the free energy must maintain the same functional form

- this implies

$$\underbrace{N\ell^{-d} f(t_\ell, h_\ell)}_{\substack{\text{free energy}\\ \text{of block spins}}} = \underbrace{N f(t,h)}_{\substack{\text{free energy}\\ \text{of spins}}} \,,$$

which yields $f(t_\ell, h_\ell) = \ell^d f(t,h)$

- we have no information how temperature and the magnetic field change during the block spin transformation
- we make the (reasonable) assumption (to be justified later)

$$t_\ell = t\,\ell^{D_t}\,, \quad D_t > 0$$

$$h_\ell = h\,\ell^{D_h}\,, \quad D_h > 0$$

$\uparrow$ dimensions of t & h

and obtain

$$f(t,h) = \ell^{-d} f(t\,\ell^{D_t}, h\,\ell^{D_h})$$

- choosing now $\ell = |t|^{-1/D_t}$, i.e. $\ell^{D_t}\, t = 1$,

we have $f(t,h) = |t|^{d/D_t} f(1, h\,|t|^{-D_h/D_t})$

- in the next step we define

$$\Delta \equiv \frac{D_h}{D_t} \quad \text{and} \quad 2-\alpha = \frac{d}{D_t},$$

which yields the scaling form of the free energy density

$$f(t,h) = |t|^{2-\alpha} F(h/t^{\Delta}),$$ which we have used already before

- this shows that the dimensions D_t and D_h are directly related to the critical exponents, e.g. $\Delta = \beta\delta$

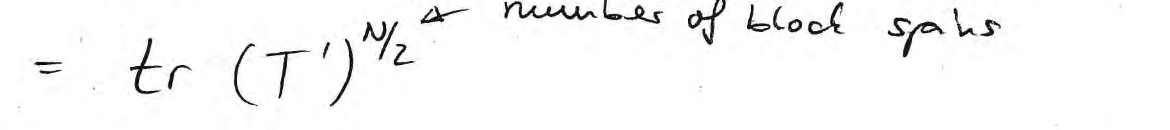
Block spin transformation in the one-dimensional Ising model

- the partition function of the one-dimensional Ising model could be expressed as the trace of the N-th power of the transfer matrix

number of spins

$$Z = \operatorname{tr} T^{N} = \operatorname{tr} \begin{pmatrix} e^{h+k} & e^{-k} \\ e^{-k} & e^{-h+k} \end{pmatrix}^{N}$$

- to conduct the block spin transformation we form blocks of neighbouring spins



- the corresponding partition function is

number of block spins

$$Z = \operatorname{tr} (T')^{N/2}$$

with $T' = T^2$

- now we write $T = \begin{pmatrix} e^{h+k} & e^{-k} \\ e^{-k} & e^{-h+k} \end{pmatrix} = \begin{pmatrix} \frac{1}{uv} & u \\ u & \frac{v}{u} \end{pmatrix}$

with $u = e^{-k}$ and $v = e^{-h}$, assuming that the parameters are such that $0 \leq u, v \leq 1$

- the transfer matrix of the block spins is then

$$T' = T^2 = \begin{pmatrix} u^2 + \frac{1}{u^2 v^2} & v + \frac{1}{v} \\ v + \frac{1}{v} & u^2 + \frac{v^2}{u^2} \end{pmatrix}$$

- we now demand that T' have the same form as T, i.e.

$$T' = c \begin{pmatrix} \frac{1}{u'v'} & u' \\ u' & \frac{v'}{u'} \end{pmatrix}.$$

Note, that this requires the introduction of an additional parameter c. Otherwise the system of equations is underdetermined.

$\hookrightarrow$ $cu' = v + \frac{1}{v}$; $\frac{c}{u'v'} = u^2 + \frac{1}{u^2 v^2}$; $\frac{cv'}{u'} = u^2 + \frac{v^2}{u^2}$

- the solution of this system of equations is

$$u' = \frac{u\sqrt{1+v^2}}{\left((u^4+v^2)(1+u^4v^2)\right)^{1/4}} \; ; \; v' = \frac{(u^4+v^2)^{1/2}}{(u^4+\frac{1}{v^2})^{1/2}}$$

$$c = \left(v + \frac{1}{v}\right)^{1/2} \left(u^4 + \frac{1}{u^4} + v^2 + \frac{1}{v^2}\right)^{1/4}$$

- by repeatedly carrying out the block spin transformation an initial point (u,v) in parameter space generates a sequence of new points
- this leads to a trajectory, and many trajectories form a flow diagram

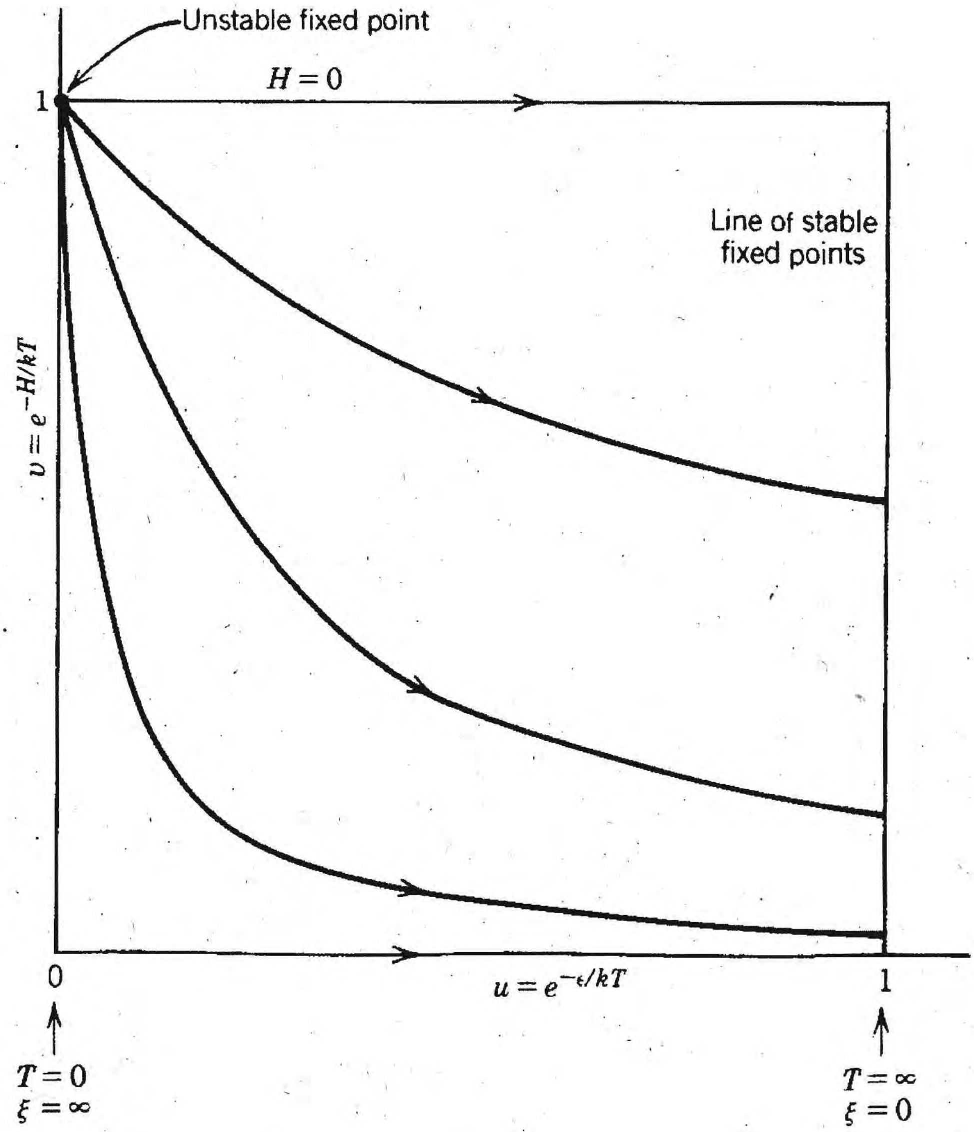


Fig. 18.3 Flow diagram of one-dimensional Ising model, showing how the coupling constant ϵ and the external field H change under successive block-spin transformations.

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- the map $R: (u,v) \to (u',v')$ has fixed points, i.e. values of u and v that do not change under the block spin transformation:

$$u = 0 \quad (\infty \text{ „interaction"}), \quad v = 1 \quad (\text{zero field})$$

and $u = 1$ (0 interaction), v arbitrary

- at the fixed points the correlation length is invariant under a change of scale and thus must be either 0 or ∞
- $u=0$ corresponds to $T=0$, where $\xi = \infty$
- $u=1$ corresponds to $T=\infty$, where $\xi = 0$
- the fixed point $(u,v) = (0,1)$ is inaccessible: either one already starts there or the flow is leading one away from it
- this is a consequence of the fact that there is no phase transition in the 1d Ising model

Fixed points and scaling fields

- the block spin transformation in the Ising model is an example of a so-called „renormalisation group" (RG) transformation

- Such RG transformation transforms the coupling constants $\vec{K}^{(n)}$ of a many-body system according to

$$\vec{K}^{(n+1)} = R(\vec{K}^{(n)})$$

coupling constants after n+1-th RG step

coupling constants after n-th RG step

- the coupling constants could e.g. be those of a general Ising model

$$\mathcal{H} = K_1 \sum_i s_i + K_2 \sum_{\langle ij \rangle} s_i s_j + K_3 \sum_{\langle\langle ij \rangle\rangle} s_i s_j + K_4 \sum_{\langle ijk \rangle} s_i s_j s_k + \ldots$$

nearest neighbours

next-nearest neighbours

- fixed points of the map R obey

$$\vec{K}^* = R(\vec{K}^*),$$

and we assume that for $n \to \infty$ $\vec{K}^{(n)}$ indeed approaches such fixed point

- at a fixed point the system is invariant under a scale change
  → ξ is either 0 or ∞ (= interesting case)
- to investigate the behaviour of the system near a fixed point, we consider $\vec{K}^{(n+1)} - \vec{K}^* = R(\vec{K}^{(n)}) - \vec{K}^*$ and make a linear approximation

$$R(\vec{K}^{(n)}) \approx \underbrace{R(\vec{K}^*) + \mathbb{W}\cdot(\vec{K}^{(n)} - \vec{K}^*)}_{\text{this is valid if } \vec{K}^{(n)} \text{ is already close to } \vec{K}^*}$$

- the matrix $\mathbb{W}$ has the entries

$$\mathbb{W}_{\alpha\beta} = \left.\frac{\partial R_\alpha(\vec{K})}{\partial K_\beta}\right|_{\vec{K}=\vec{K}^*}$$

- hence, the linearised version of the RG transformation is given by

$$\vec{K}^{(n+1)} - \vec{K}^* = \mathbb{W}(\vec{K}^{(n)} - \vec{K}^*)$$

- we now calculate the left-hand eigenvectors of $\mathbb{W}$:

$$\vec{\phi}_\mu^T \mathbb{W} = \lambda_\mu \mathbb{W}$$

- these allow us to introduce the so-called scaling fields:

$$v_\mu^{(n)} = \vec{\phi}_\mu^T (\vec{K}^{(n)} - \vec{K}^*)$$

- these scaling fields have the advantage that they do not mix under the RG transformation, which is seen as follows:

$$v_\mu^{(n+1)} = \vec{\phi}_\mu^T (\vec{K}^{(n+1)} - \vec{K}^*) = \vec{\phi}_\mu^T \mathbb{W} (\vec{K}^{(n)} - \vec{K}^*)$$

$$= \lambda_\mu \vec{\phi}_\mu^T (\vec{K}^{(n)} - \vec{K}^*) = \lambda_\mu v_\mu^{(n)}$$

- since the RG transformation increases the unit of length by a factor b, we expect the eigenvalues to be of the form $\lambda_\mu = b^{D_\mu}$
- here D_μ is referred to as the „dimension of v_μ"
- in our initial discussion of the block spins b corresponded to the linear dimension of the block spins, l
- the scaling fields were the reduced temperature, t, and the magnetic field h

- a scaling field with $\lambda_\mu < 1$ is called „irrelevant" because it tends to zero under repeated coarse graining under the RG transformation
- conversely, scaling fields with $\lambda > 1$ are „relevant" ones
- those with $\lambda = 1$ are referred to as „marginal"
- in the space of coupling constants one can define a so-called critical surface by setting all relevant scaling fields to zero : $v_\mu = 0$
- a point on the critical surface will eventually reach the fixed point under repeated RG transformations
- a point outside the surface will flow away from the fixed point
- each point on the critical surface represents a physical system, and all these systems belong to the same universality class, as they display the same critical behaviour

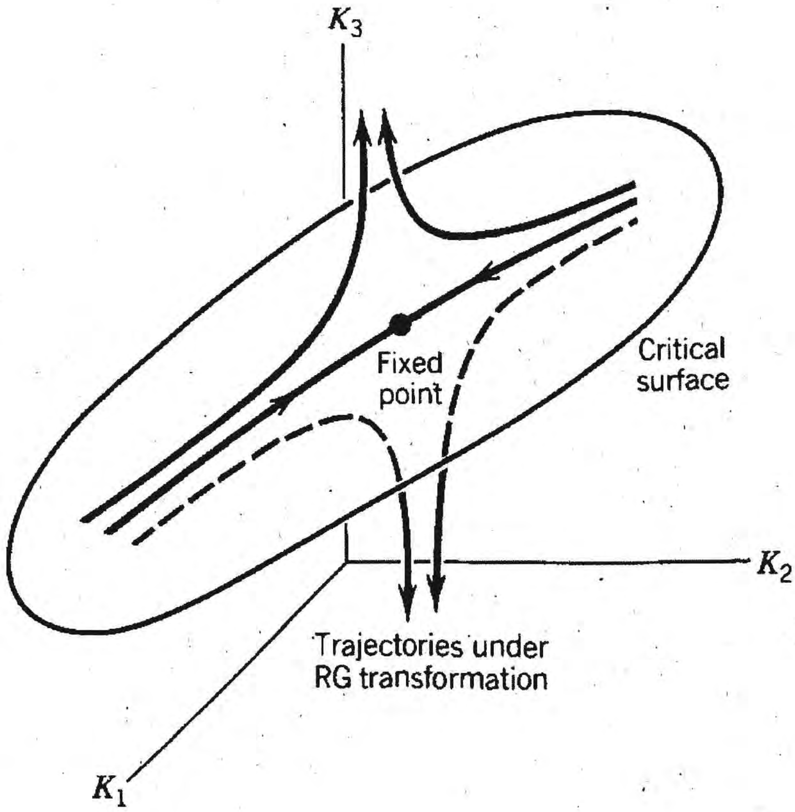

Fig. 18.4 The critical surface for a particular fixed point. It is a hypersurface in coupling-constant space obtained by setting all relevant variables to zero. Points on this surface correspond to systems in the same universality class, with the same critical exponents.

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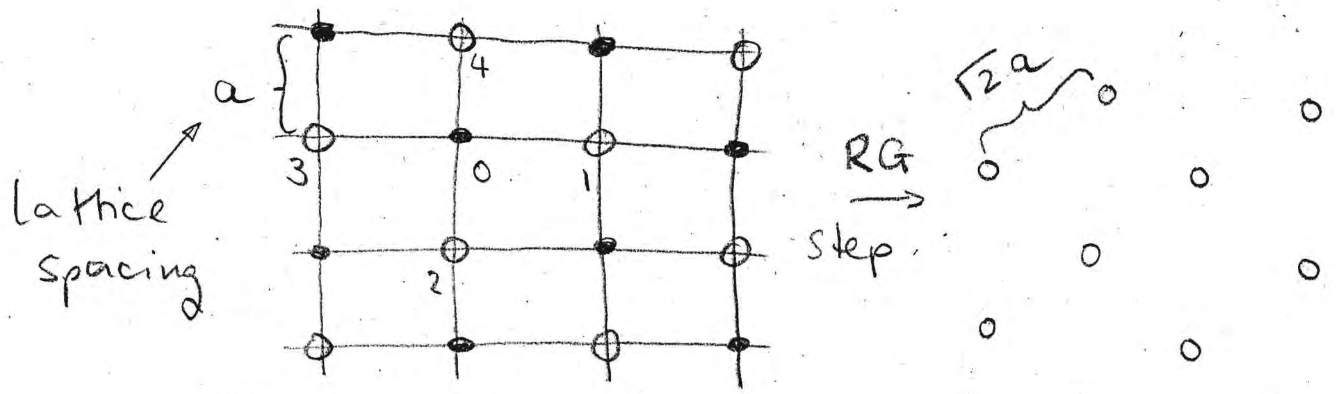
RG for the 2d Ising model on a square lattice

- we consider a square lattice, which we divide into odd and even sites



• even o odd

- we can then write the partition function of the Ising model as

$$Z = \sum_{\{S_i\}} e^{\sum_{\langle ij\rangle} K S_i S_j} = \sum_{S_j \in \text{even}} \underbrace{\sum_{S_i \in \text{odd}} e^{\sum_{\langle ij\rangle} K S_i S_j}}_{e^{-\beta \mathcal{H}(S_j)}} \qquad K = \beta\varepsilon$$

sum over all spins

sum over nearest neighbours

Ising interaction

effective Hamiltonian for the spins on the even sub-lattice

- our goal is to implement a RG transformation via a decimation procedure
- this means that we want to sum first over the odd spins, which yields a new Hamiltonian with modified coupling constants for the even spins
- the even spins, however, also form a 2d square lattice and thus the system looks the same as before
- the only differences are that the lattice is rotated by 45° and that the new lattice constant is $\sqrt{2}\, a$ instead of a
- unlike for the 1d Ising model, the RG transformation cannot be done exactly, i.e. the new Hamiltonian does not have the same form as the original one, unless one makes some approximations

- for the decimation procedure we need to compute terms of the type

$$z_0 = \sum_{S_0=\pm 1} \exp\left[K S_0 (S_1 + S_2 + S_3 + S_4)\right]$$

- quite generally, this function can be written in the form (will be shown on next page)

$$Z_0 = \exp\Big[A\overbrace{(S_1S_2 + S_2S_3 + S_3S_4 + S_1S_4)}^{\text{nearest neighbour terms}} + B\overbrace{(S_1S_3 + S_2S_4)}^{\text{next nearest neighbour terms}} + C\, S_1S_2S_3S_4 + D\Big]$$

- the problem is now, that this form is different from the original one, e.g. because it involves 4-body interactions
- we thus have to make a crude approximation, making the modification

$$Z_0 \to \overline{Z_0} = \exp\Big[(A + \underbrace{\tfrac{B}{2}}_{\text{factor } \frac{1}{2} \text{ to account for relative numbers of terms}})(S_1S_2 + S_2S_3 + S_3S_4 + S_1S_4) + D\Big]$$

- in the full partition function a term, such as $\exp\left[(A+\frac{B}{2})S_1S_2\right]$ will be generated from two odd sites

- this is why $A + \frac{B}{2} = \frac{K_1}{2}$, where K_1 is the coupling constant between the spins after the RG step

- the final task is to find the values of the coefficients A, B, C, D, which is done by comparing the 2 expressions for Z_0:

$$
\begin{array}{lcl|cccc}
 & & & s_1 & s_2 & s_3 & s_4 \\
2 & = & e^{(-4A+2B+C+D)} & +1 & -1 & +1 & -1 \\
2 & = & e^{(-2B+C+D)} & +1 & +1 & -1 & -1 \\
e^{4K}+e^{-4K} & = & e^{(4A+2B+C+D)} & +1 & +1 & +1 & +1 \\
e^{2K}+e^{-2K} & = & e^{(-C+D)} & +1 & +1 & +1 & -1
\end{array}
$$

- these yield $A = B = \frac{1}{8}\log(\cosh(4K))$, and we find that the old and new coupling constants are related through $K_1 = 2A+B = \frac{3}{8}\log(\cosh(4K))$

$$= R(K)$$

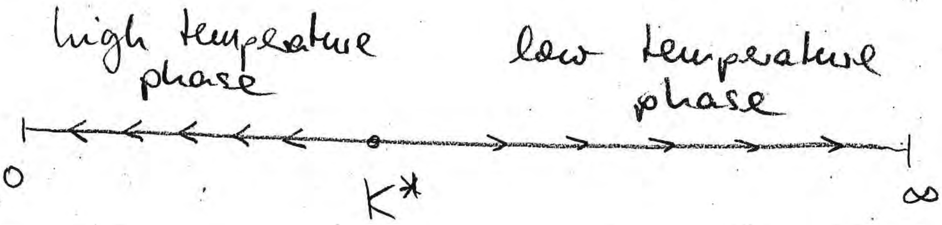
- this map has a fixed point at $K^* = 0.507$, which marks the critical coupling strength

- comparing with the exact solution of the 2d Ising model:

$$K^*_{2d\,\text{Ising}} = \varepsilon \beta_c = \frac{\log(1+\sqrt{2})}{2} = 0.441$$

the agreement is remarkably good

- if the map R is iterated K values that lie below K^* will move towards zero, while initial values of K, which are larger than K^* move towards infinity



- all systems with coupling constants below (above) K^* belong to the high (low) temperature phase

- in the vicinity of the critical point, we can expand the map linearly, yielding

$$K^{(n+1)} - K^* = \left.\frac{\partial R(K)}{\partial K}\right|_{K=K^*} (K^{(n)} - K^*)$$

and hence $\left.\frac{\partial R(K)}{\partial K}\right|_{K=K^*} = 1.449$ is the eigenvalue λ corresponding to the scaling field $\bar{K} = K - K^*$

- we can now calculate the dimension of the scaling field by realising that in each RG step the unit of length increases by $b = \sqrt{2}$

↳ $\lambda = \sqrt{2}^{D_{\bar{K}}}$ → $D_{\bar{K}} = \frac{\log \sqrt{2}}{\log 1.449} = 0.935$

- hence $\bar{K} \sim \xi^{D_{\bar{K}}}$, and since $\bar{K} \sim \frac{1}{|t|}$, one finds $|t| \sim \xi^{-D_{\bar{K}}}$ and therefore $D_{\bar{K}} = \frac{1}{\nu}$
- the agreement with the exact value $\nu = 1$ is again remarkably good ($\frac{1}{D_{\bar{K}}} \approx 1.07$)

Bose - Einstein Condensation Summary

- single particle energies:

$$\varepsilon_{\vec{p}} = \frac{\vec{p}^2}{2m} = \frac{\hbar^2 \vec{k}^2}{2m} = \varepsilon_p$$

- mean occupation number

$$\overline{n}_p = \frac{1}{e^{\beta(\varepsilon_p - \mu)} - 1}$$

μ: chemical potential

- total number of bosons

$$N = N_0 + \sum_{\vec{p} \neq 0} \overline{n}_p = N_0 + \frac{V}{(2\pi\hbar)^3} \int d^3\vec{p}\ \overline{n}_p$$

$$= N_0 + \frac{V}{\lambda^3}\, g_{3/2}(z)$$

N_0: number of bosons in ground state

$\sum_{\vec{p} \neq 0} \overline{n}_p$: bosons populating excited states

λ: thermal wave length $\lambda = \frac{2\pi\hbar}{\sqrt{2\pi m k_B T}}$

z: fugacity $z = e^{\beta\mu}$

$g_{3/2}$: generalised Riemann Zeta function $g_\nu(z) = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell^\nu}$

condensation

- below the critical temperature the chemical potential must be zero (otherwise the mean occupation number can diverge)

- at this point one has

$$\mu = 0 \rightarrow z = 1 \rightarrow g_{3/2}(1) = \underbrace{\zeta\left(\tfrac{3}{2}\right)}_{\substack{\text{Riemann} \\ \text{zeta function}}}$$

$$\zeta(\nu) = \sum_{l=1}^{\infty} \frac{1}{l^\nu}$$

- below the critical temperature one thus has

$$N = N_0 + \frac{V}{\lambda^3}\zeta\left(\tfrac{3}{2}\right) = N_0 + \frac{\lambda_c^3}{\lambda^3}\frac{V}{\lambda_c^3}\zeta\left(\tfrac{3}{2}\right)$$

$$= N_0 + \left(\frac{T}{T_c}\right)^{3/2} \underbrace{\frac{V}{\lambda_c^3}\zeta\left(\tfrac{3}{2}\right)}_{\substack{\text{at the} \\ \text{critical} \\ \text{point}}} = N_0 + N\left(\frac{T}{T_c}\right)^{3/2}$$

point $N_0 = 0 \rightarrow \frac{V}{\lambda_c^3}\zeta\left(\frac{3}{2}\right) = N$

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}^{+}(\vec{r}\,')\right] = \frac{1}{\cancel{\;}V}\sum_{kk'} \underbrace{[a_k, a_{k'}^{+}]}_{\delta_{kk'}} e^{-i\vec{k}\cdot\vec{r} + i\vec{k}'\cdot\vec{r}\,'}$$

$$= \frac{1}{\cancel{\;}V}\sum_{k} e^{-i\vec{k}(\vec{r}-\vec{r}\,')} = \delta(\vec{r}-\vec{r}\,')$$

$$\frac{1}{V}\int d^3\vec{r}\, \frac{\hbar^2}{2m}|\vec{k}|^2 \sum_{k'k} a_{k'}^{+} a_k\, e^{i\cancel{\;} r(k'-k)}$$

$$= \sum_{kk'} \frac{\hbar^2 |\vec{k}|^2}{2m} a_{k'}^{+} a_k \underbrace{\frac{1}{V}\int d^3\vec{r}\, e^{ir(k'-k)}}_{\frac{1}{V} V \delta_{k'k}}$$

$$\frac{1}{V^2}\int d^3 r \sum_{kk'qq'} a_k^{+} a_q^{+} a_{k'} a_{q'}\, e^{i\vec{r}(k+q-k'-q')}$$

$$q' = k + q - k'$$

$$H = \sum_k \varepsilon_k a_k^+ a_k + \frac{U_0}{2V}\left[N_0^2 + N_0 \sum_k \left(a_k a_{-k} + a_k^+ a_{-k}^+ + 2a_k^+ a_k + 2a_{-k}^+ a_{-k}\right)\right]$$

$$\approx \sum_k \varepsilon_k a_k^+ a_k + \frac{U_0}{2V}\Big[N^2 - N \sum_k \left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)$$

$$+ N \sum_k \left(a_k a_{-k} + a_k^+ a_{-k}^+\right)$$

$$+ 2N \sum_k \left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)\Big]$$

$$= \frac{1}{2} \sum_k{}' \left(\varepsilon_k + \frac{U_0 N}{2V}\right)\left(a_k^+ a_k + a_{-k}^+ a_{-k}\right)$$

$$+ \sum_k \frac{U_0 N}{2V}\left(a_k a_{-k} + a_k^+ a_{-k}^+\right) + \frac{U_0 N}{2V}$$

$$\frac{\varepsilon_1}{\varepsilon_0} = \frac{2 \sinh t \cosh t}{\cosh^2 t + \sinh^2 t} = \frac{\sinh 2t}{\cosh 2t}$$

$$= \tanh 2t$$

$$u^2 = \cosh^2 t \qquad \text{Solve together} \qquad u^2 = 1 + v^2$$

$$\frac{\varepsilon_1}{\varepsilon_0} = \frac{2uv}{u^2+v^2} = \frac{(u+v)^2 - u^2 - v^2}{u^2+v^2} = \frac{(u+v)^2}{u^2+v^2} - 1$$

$$= \frac{2uv}{1+2v^2} = \frac{2\sqrt{1+v^2}\, v}{1+2v^2} \rightarrow \left(\frac{\varepsilon_1}{\varepsilon_0}\right)^2 = \frac{4(1+v^2)v^2}{(1+2v^2)^2}$$

The weakly interacting Bose gas

- a system of non interacting bosons undergoes at sufficiently low temperature a phase transition into a Bose-Einstein condensate

- for a homogeneous system this means that the state with zero momentum (ground state) becomes macroscopically occupied

number of bosons in zero momentum mode

$$\frac{N_0}{N} = \begin{cases} 1-\left(\frac{T}{T_c}\right)^{3/2} & ; \quad T < T_c \\ 0 & ; \quad T > T_c \end{cases}$$

total number of bosons

- the critical temperature at which this transition takes place is

volume

$$k_B T_c = \frac{2\pi}{\left[\zeta\left(\frac{3}{2}\right)\right]^{2/3}} \frac{\hbar}{m \left(\frac{V}{N}\right)^{2/3}}$$

Riemann zeta function

mass of boson

- we are now interested in investigation the impact of interactions between bosons (near $T=0$)

- the Hamilton for interacting bosons is given by

$$\mathcal{H} = \int d^3\vec{r} \left[-\hat{\psi}^+(\vec{r}) \frac{\hbar^2}{2m} \nabla^2 \hat{\psi}(\vec{r}) \right]$$

annihilation operator of boson at position $\vec{r}\,'$

$$+ \frac{1}{2} \int d^3\vec{r}\, d^3\vec{r}\,' \, \hat{\psi}^+(\vec{r})\, \hat{\psi}^+(\vec{r}\,')\, V(|\vec{r}-\vec{r}\,'|)\, \hat{\psi}(\vec{r}\,')\, \hat{\psi}(\vec{r})$$

interaction potential between bosons

- field operators obey
$[\hat{\psi}(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = \delta(\vec{r}-\vec{r}\,')$
$[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')] = [\hat{\psi}^+(\vec{r}), \hat{\psi}^+(\vec{r}\,')] = 0$

- to simplify the situation we replace the real interaction by a so-called contact interaction: $V(\vec{r}) \approx U_0\, \delta(\vec{r})$.

- this means that two particles interact only when they are at the same position, and their interaction strength is given by U_0

- note, that such approximate description is valid only at low energies (momenta) of the bosons; for high momenta a so-called regularisation is required

- using the contact interaction, the Hamiltonian becomes

$$\mathcal{H} = \int d^3\vec{r} \left[-\hat{\psi}^+(\vec{r}) \frac{\hbar^2}{2m} \nabla^2 \hat{\psi}(\vec{r}) + \frac{U_0}{2} \hat{\psi}^+(\vec{r}) \hat{\psi}^+(\vec{r}) \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r}) \right]$$

- using plane waves as a basis for representing the field operators,

$$\hat{\psi}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} a_{\vec{k}} e^{-i\vec{k}\vec{r}}, \quad \hat{\psi}^+(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{k}} a^+_{\vec{k}} e^{i\vec{k}\vec{r}},$$

where the $a_{\vec{k}}$ are bosonic operators, i.e. $[a_{\vec{k}}, a^+_{\vec{q}}] = \delta_{\vec{k}\vec{q}}$, we can write

$$\mathcal{H} = \sum_{\vec{k}} \underbrace{\frac{\hbar^2 |\vec{k}|^2}{2m}} a^+_{\vec{k}} a_{\vec{k}} + \frac{U_0}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3} a^+_{\vec{k}_1} a^+_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1 + \vec{k}_2 - \vec{k}_3}$$

ε_k ... energy for creating a boson with momentum $k = |\vec{k}|$

- close to $T=0$, which certainly is below T_c, the mode with $\vec{k}=0$ is macroscopically occupied
- therefore we approximate the bosonic operators associated with this mode by numbers

$\hookrightarrow \quad a_0^+ \longrightarrow \sqrt{V}\,\phi_0 \quad , \quad a_0 \longrightarrow \sqrt{V}\,\phi_0^*$

- with this replacement we can write for the condensed fraction of atoms by

$$\frac{N_0}{V} = |\phi_0|^2$$

- using this approximation, and furthermore assuming that the occupation of modes with $\vec{k} \neq 0$ is small, we can also approximate,

$$\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3} a^+_{\vec{k}_1} a^+_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_1+\vec{k}_2-\vec{k}_3} \approx \overbrace{V^2 |\phi_0|^4}^{\text{zero momentum components}} +$$

$$+ V \sum_{\vec{k}}{}' \underbrace{\left[\phi_0^{*2} a_{\vec{k}} a_{-\vec{k}} + \phi_0^2 a^+_{\vec{k}} a^+_{-\vec{k}} + 2|\phi_0|^2 (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a^+_{-\vec{k}}) \right]}$$

summation only over modes with $\vec{k} \neq 0$.

all quartic terms have been omitted, since population of these modes is assumed to be small ($\langle a^+_k a^+_p a_q a_m \rangle \ll N_0^2$)

- in the next step we make the simplifying assumption that $\phi_0 \in \mathbb{R}$ and exploit the conservation of the number of particles:

$$N = N_0 + \frac{1}{2} \sum_{\vec{k}}{}' (a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}})$$

N: total number of particles; N_0: number of particles in condensate

- using that $N \gg \langle a^+_{\vec{k}} a_{\vec{k}} \rangle$ we can approximate

$$N_0^2 = \left(N - \frac{1}{2} \sum_{\vec{k}}{}' \left(a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}} \right) \right)^2$$

$$\simeq N^2 - N \sum_{\vec{k}}{}' \left(a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}} \right)$$

note, that we have here replaced to operator N by a number, i.e. its average value

- this allows us to eliminate

$$V |\phi_0|^2 = V \phi_0^{*2} = V \phi_0^2 = N_0$$

from the Hamiltonian, which then takes the form

$$\mathcal{H} = \frac{U_0 N^2}{2V} + \frac{1}{2} \sum_{\vec{k}}{}' \Big[\left(\varepsilon_k + U_0 \frac{N}{V} \right) \left(a^+_{\vec{k}} a_{\vec{k}} + a^+_{-\vec{k}} a_{-\vec{k}} \right)$$
$$+ U_0 \frac{N}{V} \left(a_{\vec{k}} a_{-\vec{k}} + a^+_{\vec{k}} a^+_{-\vec{k}} \right) \Big]$$

- note, that this Hamiltonian is only valid, when $N_0 \simeq N \gg \langle a^+_{\vec{k}} a_{\vec{k}} \rangle$

- the Hamiltonian is a quadratic form and therefore can be diagonalised analytically

- this achieved by a <u>Bogoliubov transformation</u>
- this is similar to what we did in the context of solving the quantum Ising model with a transverse field
- however, since we are here dealing with bosons, there are some differences compared to the quantum Ising model which was mapped onto fermions
- the Hamiltonian is a sum of terms of the type

$$h = \varepsilon_0 (a^+ a + b^+ b) + \varepsilon_1 (a^+ b^+ + b a)$$

- we seek new bosonic operators (α, β) which bring this Hamiltonian into a canonical form (not containing terms of the type $\alpha^+ \beta^+$)
- we make the ansatz

coefficients (assumed to be real)

$$\alpha = u a + v b^+ \, , \quad \beta = u b + v a^+$$

and require canonical commutation relations:

$$[\alpha, \alpha^+] = [\beta, \beta^+] = 1 \, , \quad [\alpha, \beta^+] = [\alpha, \beta] = 0$$

- we find

$$[\alpha, \alpha^+] = [ua + vb^+, ua^+ + vb] = u^2 \underbrace{[a, a^+]}_{=1} + v^2 \underbrace{[b^+, b]}_{=-1} \overset{!}{=} 1$$

- hence, the coefficients u and v have to obey $u^2 - v^2 = 1$
- note, that this is different compared to fermions, where we found a relative '+' sign
- the inverse transformation is

$$a = u\alpha - v\beta^+ \quad , \quad b = u\beta - v\alpha^+$$

and inserting it into the Hamiltonian h, yields

$$h = 2v^2 \varepsilon_0 - 2uv\varepsilon_1 + [\varepsilon_0 (u^2 + v^2) - 2uv\varepsilon_1](\alpha^+\alpha + \beta^+\beta)$$

$$+ \underbrace{[\varepsilon_1 (u^2 + v^2) - 2uv\varepsilon_0]}_{\text{we require this to be zero}}(\alpha\beta + \alpha^+\beta^+)$$

- parameterising $u = \cosh t$, $v = \sinh t$, which automatically imposes $u^2 - v^2 = 1$, we find

$$\varepsilon_1 (u^2 + v^2) - 2uv\varepsilon_0 = \varepsilon_1 (\cosh^2 t + \sinh^2 t) - 2\varepsilon_0 \sinh t \cosh t = 0$$

- This yields $\tanh 2t = \frac{\varepsilon_1}{\varepsilon_0}$ and leads to

$$u^2 = \frac{1}{2}\left(\frac{\varepsilon_0}{\varepsilon} + 1\right) \quad \text{and} \quad v^2 = \frac{1}{2}\left(\frac{\varepsilon_0}{\varepsilon} - 1\right)$$

with $\varepsilon = \sqrt{\varepsilon_0^2 - \varepsilon_1^2}$

- This leads to the diagonalised form of the Hamiltonian:

$$h = \varepsilon(\alpha^+\alpha + \beta^+\beta) + \varepsilon - \varepsilon_0$$

- applying these results to the BEC Hamiltonian yields

$$a_{\vec{k}} = u_{\vec{k}}\alpha_{\vec{k}} - v_{\vec{k}}\alpha^+_{-\vec{k}} \quad , \quad a_{-\vec{k}} = u_{-\vec{k}}\alpha_{-\vec{k}} - v_{\vec{k}}\alpha^+_{\vec{k}}$$

$$\hookrightarrow \mathcal{H} = \frac{U_0 N^2}{2V} - \frac{1}{2}\sum_{\vec{k}}{}' \left(\varepsilon_k + U_0\frac{N}{V} - E_k\right) + \frac{1}{2}\sum_{\vec{k}}{}' E_k\left(\alpha^+_{\vec{k}}\alpha_{\vec{k}} + \alpha^+_{-\vec{k}}\alpha_{-\vec{k}}\right)$$

with $E_k = \sqrt{\varepsilon_k\left(\varepsilon_k + 2U_0\frac{N}{V}\right)}$ } excitation spectrum of the BEC

and
$$u^2_{\vec{k}} = u^2_k = \frac{1}{2}\left[\frac{\varepsilon_k + U_0\frac{N}{V}}{E_k} + 1\right]$$

$$v^2_{\vec{k}} = v^2_k = \frac{1}{2}\left[\frac{\varepsilon_k + U_0\frac{N}{V}}{E_k} - 1\right]$$

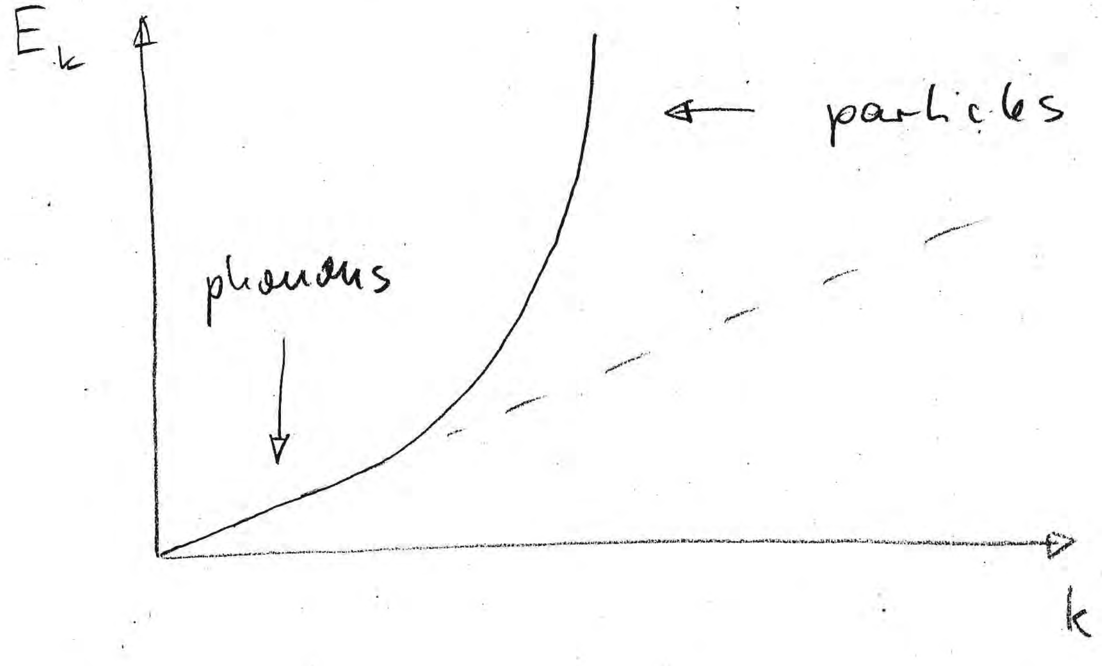
- this result shows, that for small wave vectors, where $\varepsilon_k \ll 2U_0 \frac{N}{V}$, the dispersion relation is approximately linear

  ↳ $E_k \approx \hbar c |k|$ where $c = \sqrt{\frac{U_0 N}{mV}}$

  can be interpreted as the sound velocity of the elementary (quasi-particle) excitations, which are phonons

- conversely, when $\varepsilon_k \gg 2U_0 \frac{N}{V}$ the dispersion relation becomes

  $E_k \approx \frac{\hbar^2 k^2}{2m}$ and the elementary excitations are particles with mass m



- with these results one can show that interactions actually reduce the number of particles in the condensate, which is referred to as <u>condensate depletion</u>

- to see this we express the particle number in terms of the quasi particle creation and annihilation operators

$$N = N_0 + \sum_{\vec{k}}{}' v_k^2 + \sum_{\vec{k}}{}' (u_k^2 + v_k^2)\, \alpha_{\vec{k}}^+ \alpha_{\vec{k}} - \sum_{\vec{k}}{}' u_k v_k \left(\alpha_{\vec{k}}^+ \alpha_{-\vec{k}}^+ + \alpha_{-\vec{k}} \alpha_{\vec{k}}\right)$$

- at zero temperature no quasi-particles will be excited and the BEC is in its ground state: $|0\rangle$ with $\alpha_k |0\rangle = 0$

- hence, $\underbrace{\langle N\rangle - N_0}_{\text{number of particles not in the ground state}} = \langle 0|N|0\rangle - N_0 = \sum_{\vec{k}}{}' v_k^2$

$$= V \int \frac{d^3\vec{k}}{(2\pi)^3}\, v_k^2 = \frac{V}{(2\pi)^3} \cdot 4\pi \int_0^\infty dk\, k^2\, v_k^2$$

$$= \frac{V}{2\pi^2} \int_0^\infty dk\, k^2 \left(\frac{\frac{\hbar^2 k^2}{2m} + U_0 \frac{N}{V}}{\left[\frac{\hbar^2 k^2}{2m}\left(\frac{\hbar^2 k^2}{2m} + 2U_0 \frac{N}{V}\right)\right]^{1/2}} - 1 \right)$$

$$= \frac{V}{2\pi^2} \int_0^\infty dk\, k^2 \frac{k^2+\gamma}{\sqrt{k^2(k^2+2\gamma)}} = \frac{V}{6\pi^2} \sqrt{2}\, \gamma^{3/2}$$

with $\gamma = \frac{2m U_0}{\hbar^2} \frac{N}{V}$

$$\hookrightarrow \underbrace{\frac{\langle N \rangle - N_0}{N}}_{\substack{\text{fraction of}\\ \text{atoms outside}\\ \text{the condensate}}} = \frac{N-N_0}{N} = \frac{1}{3\pi} \sqrt{\frac{m^3 U_0^3}{\hbar^3} \frac{N}{V}}$$

- finally, we consider the ground state energy of the condensate and how it is changed by interactions
- this can in principle be calculated via

$$E_0 = \langle 0 | \mathcal{H} | 0 \rangle = \frac{U_0 N^2}{2V} - \frac{1}{2} \sum_{\vec{k}}{}' \left(\varepsilon_k + U_0 \frac{N}{V} - E_k \right)$$

- however, the sum over the momenta is divergent, which stems from the fact that the contact interaction, as we used it, is incorrect for high momenta

- when treating the contact interaction in a way that is consistent also for high momenta, one obtains

$$E_0 = \frac{U_0 N^2}{2V} - \frac{1}{2}\sum_{\vec{k}}\left[\varepsilon_k + U_0\frac{N}{V} - E_k - \underbrace{\frac{1}{2\varepsilon_k}\left(\frac{U_0 N}{V}\right)^2}_{\substack{\text{term, which}\\ \text{regularises}\\ \text{divergence of}\\ \text{the sum}}}\right]$$

- converting the sum to an integral then leads to the following expression for the energy density of the ground state:

$$\frac{E_0}{V} = \frac{U_0 N^2}{2V^2} + \frac{8}{15\pi^2}\left(\frac{\sqrt{m}}{\hbar}\right)^3\left(U_0\frac{N}{V}\right)^{5/2}$$

Dynamics of the Ising model

- So far we have only discussed the properties of the canonical (thermal) state of the Ising model
- here the probability to find the system in a microstate $\{S_i\} \equiv \underline{S}$ given by

$$p_{th}(\underline{S}) = \frac{e^{-\beta E\{S_i\}}}{Z} = \frac{e^{-\beta E(\underline{S})}}{Z}$$

where $E\{S_i\}$ is the energy of the microstate / spin configuration and Z the partition function

- Statistical mechanics does not have a prescription concerning the dynamics, unlike quantum mechanics, where the Hamiltonian determines both the energetics and the temporal evolution

- a way for modelling the dynamics of the thermal Ising model is through a rate equation of the form (so called Markovian master equation)

$$\frac{\partial p(\underset{\sim}{S},t)}{\partial t} = \sum_{\underset{\sim}{S}'} \left[W_{\underset{\sim}{S}\underset{\sim}{S}'} \, p(\underset{\sim}{S}',t) - W_{\underset{\sim}{S}'\underset{\sim}{S}} \, p(\underset{\sim}{S},t) \right]$$

- here $W_{\underset{\sim}{S}\underset{\sim}{S}'}$ is the transition rate between two microstates $\underset{\sim}{S}$ and $\underset{\sim}{S}'$, eg.

$$\underbrace{\uparrow \downarrow \uparrow \uparrow \downarrow \uparrow}_{\underset{\sim}{S}} \xrightarrow{W_{\underset{\sim}{S}\underset{\sim}{S}'}} \underbrace{\uparrow \downarrow \downarrow \uparrow \downarrow \uparrow}_{\underset{\sim}{S}'}$$

which corresponds to a single spin flip

- the stationary state of the master equation is defined by $\frac{\partial p(\underset{\sim}{S},t)}{\partial t} = 0$

$$\hookrightarrow \sum_{\underset{\sim}{S}'} \left[W_{SS'} \, p(\underset{\sim}{S}',t) - W_{\underset{\sim}{S}'\underset{\sim}{S}} \, p(\underset{\sim}{S},t) \right] = 0,$$

which needs to be satisfied for all microstates $\underset{\sim}{S}$

- note, that stationarity merely requires the sum over all terms to be zero, i.e. the net flow of probability between each microstate ξ' and all other states vanishes
- a particular solution is given by the case in which all terms of the sum exactly cancel

↳ $w_{\xi\xi'}\, p_{eq}(\xi') = w_{\xi'\xi}\, p_{eq}(\xi)$ for all ξ, ξ'

- this condition is called detailed balance, and a state (probability distribution) that satisfies

$$\frac{p_{eq}(\xi)}{p_{eq}(\xi')} = \frac{w_{\xi\xi'}}{w_{\xi'\xi}}$$

is called an equilibrium state

- therefore, in order to obtain a stationary state, that is the canonical state, we have to choose the rates according to

$$\frac{w_{\xi\xi'}}{w_{\xi'\xi}} = \frac{p_{th}(\xi)}{p_{th}(\xi')} = \frac{e^{-\beta E(\xi)}}{e^{-\beta E(\xi')}} = e^{-\beta(E(\xi)-E(\xi'))}$$

- this condition fixes only the ratio of the rates
- therefore, there is a lot of freedom in choosing the rates; e.g. we can multiply them by a constant or even a function of the spin configuration, and still the stationary state would remain (in principle) the same
- the simplest dynamics is the so-called <u>Glauber dynamics</u> which consists of single spin flips

↳

$$\underset{k}{\downarrow\ \uparrow\ \downarrow} \quad \underset{\Gamma_k^+}{\overset{\Gamma_k^-}{\rightleftarrows}} \quad \underset{k}{\downarrow\ \downarrow\ \downarrow}$$

with rates: $$\Gamma_k^{\pm} = \frac{e^{\pm\beta\varepsilon(s_{k-1}+s_{k+1})}}{e^{\beta\varepsilon(s_{k-1}+s_{k+1})}+e^{-\beta\varepsilon(s_{k-1}+s_{k+1})}}$$

$$= \frac{1}{2}\left(1 \pm \tanh\left(\beta\varepsilon(s_{k-1}+s_{k+1})\right)\right)$$

possible, because $s_{k\pm1}$ only take values -1 and $+1$ ⟶ $$= \frac{1}{2}\left(1 \pm \frac{1}{2}(s_{k-1}+s_{k+1})\tanh(2\beta\varepsilon)\right)$$

- when $T \to 0$, i.e. $\beta \to \infty$ these rates become particularly simple:

$$\Gamma_k^{\pm} \xrightarrow{\beta \to \infty} \frac{1}{2}\left(1 \pm \frac{1}{2}(S_{k-1} + S_{k+1})\right)$$

- here only spin flips, that lower or conserve the energy can take place

$$\uparrow\downarrow\uparrow \quad \begin{array}{c} \longrightarrow \\ \cancel{\longleftarrow} \end{array} \quad \uparrow\uparrow\uparrow$$

$$\uparrow\downarrow\downarrow \quad \begin{array}{c} \longrightarrow \\ \longleftarrow \end{array} \quad \uparrow\uparrow\downarrow$$

- let us now investigate, how the dynamics of observables, such as the magnetisation or correlation functions can be calculated with the help of the master equations

- to this end it is actually convenient to introduce a bra-ket notation like usually in quantum mechanics

- introducing the probability vector

$$|p\rangle = \sum_{s_1 \dots s_N = \pm 1} p_{s_1 s_2 \dots s_N} |s_1\rangle |s_2\rangle \dots |s_3\rangle, \text{ with } |s_j\rangle = \begin{cases} |1\rangle \\ |-1\rangle \end{cases}$$

allows us to write the master equation as

$\partial_t |p) = W|p)$, where W is the so-called dynamical or master operator

- an important role in this formulation plays the reference vector

$$|\mathbb{1}\rangle = \sum_{s_1 \ldots s_N = \pm 1} |s_1) \ldots |s_N) = (|1)_1 + |-1)_1)(|1)_2 + |-1)_2) \ldots (|1)_N + |-1)_N)$$

with the help of which we can write the normalisation condition $\langle \mathbb{1}|p\rangle = 1$ (sum over all probabilities is one)

- this also implies $\underbrace{\partial_t \langle \mathbb{1}|p\rangle}_{0} = \langle \mathbb{1}|W|p\rangle \rightarrow \langle \mathbb{1}|W|p\rangle = 0$

and hence $\langle \mathbb{1}|W = 0$, i.e. $\langle \mathbb{1}|$ is a left-eigenvector of W with eigenvalue 0 (all columns of W sum up to zero)

- the expectation value of a quantity X is calculated according to $\langle X\rangle = \langle \mathbb{1}|X|p\rangle$

- the dynamical operator of the 1d Ising model under Glauber dynamics is

$$W = \sum_{k=1}^{N} \left[\Gamma_k^+ \left(\overbrace{\sigma_k^+}^{\begin{pmatrix}0&1\\0&0\end{pmatrix}} - \overbrace{\sigma_k^- \sigma_k^+}^{\begin{pmatrix}0&0\\0&1\end{pmatrix}} \right) + \Gamma_k^- \left(\overbrace{\sigma_k^-}^{\begin{pmatrix}0&0\\1&0\end{pmatrix}} - \overbrace{\sigma_k^+ \sigma_k^-}^{\begin{pmatrix}1&0\\0&0\end{pmatrix}} \right) \right]$$

$$= \sum_{k=1}^{N} \begin{pmatrix} -\Gamma_k^- & \Gamma_k^+ \\ \Gamma_k^- & -\Gamma_k^+ \end{pmatrix}_k , \quad \text{with } \Gamma_k^{\pm} = \frac{1}{2}\left(1 \pm \frac{1}{2}(\sigma_z^{k-1} + \sigma_z^{k+1}) \tanh(2\beta\varepsilon)\right)$$

- the time evolution of the expectation value of the magnetisation of the m-th spin is then calculated according to

$$\langle \mathbb{1} | \sigma_z^m \partial_t | p \rangle = \partial_t \langle \sigma_z^m \rangle = \partial_t M_m$$

$$= \langle \mathbb{1} | \sigma_z^m W | p \rangle$$

$$= \underbrace{\langle \mathbb{1} | \sigma_z^m \begin{pmatrix} 0 & 1 \\ 0 & -1 \end{pmatrix}_m}_{\langle \mathbb{1} | (1 - \sigma_z^m)} \Gamma_m^+ | p \rangle + \underbrace{\langle \mathbb{1} | \sigma_z^m \begin{pmatrix} -1 & 0 \\ 1 & 0 \end{pmatrix}_m}_{- \langle \mathbb{1} | (1 + \sigma_z^m)} \Gamma_m^- | p \rangle$$

$$= - \underbrace{\langle \sigma_z^m \rangle}_{M_m} + \frac{1}{2} \underbrace{\langle (\sigma_z^{m-1} + \sigma_z^{m+1}) \rangle}_{M_{m-1} + M_{m+1}} \tan(2\beta\epsilon)$$

- at $T = 0$ this becomes

$$\partial_t M_m(t) = - M_m(t) + \frac{1}{2} \left(M_{m-1}(t) + M_{m+1}(t) \right)$$

which describes the evolution of the magnetisation as a function of time

$$\langle \mathbb{1} | \sigma_z^m W | p\rangle = \sum_k \langle \mathbb{1} | \sigma_z^m \Gamma_k^+ (\sigma_k^+ - \sigma_k^- \sigma_k^+) | p\rangle$$

$$+ \sum_k \langle \mathbb{1} | \sigma_z^m \Gamma_k^- (\sigma_k^- - \sigma_k^+ \sigma_k^-) | p\rangle$$

$$= \sum_{k\neq m} \underbrace{\langle \mathbb{1} | \Gamma_k^+ (\sigma_k^+ - \sigma_k^- \sigma_k^+)}_{} \sigma_z^m | p\rangle + \sum_{k\neq m} \langle \mathbb{1} | \Gamma_k^- (\sigma_k^- - \sigma_k^+ \sigma_k^-) \sigma_z^m | p\rangle$$

$$\begin{pmatrix}1\\1\end{pmatrix}_1^T \otimes \dots \otimes \underbrace{\begin{pmatrix}1\\1\end{pmatrix}_k^T \begin{pmatrix}0 & \Gamma_k^+\\ 0 & -\Gamma_k^+\end{pmatrix}_k}_{0} \otimes \otimes \begin{pmatrix}1\\1\end{pmatrix}^T \sigma_z^m \otimes \dots \otimes | p\rangle$$

$$+ \langle \mathbb{1} | \underbrace{\sigma_z^m \Gamma_m^+ (\sigma_m^+ - \sigma_m^- \sigma_m^+)}_{} | p\rangle + \langle \mathbb{1} | \sigma_z^m \Gamma_m^- (\sigma_m^- - \sigma_m^+ \sigma_m^-) | p\rangle$$

$$\begin{pmatrix}1\\1\end{pmatrix}^T \underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \begin{pmatrix}0 & \Gamma_m^+\\ 0 & -\Gamma_m^+\end{pmatrix}}_{}$$

$$\begin{pmatrix}1\\-1\end{pmatrix}^T \begin{pmatrix}0 & \Gamma_m^+\\ 0 & -\Gamma_m^+\end{pmatrix} = \begin{pmatrix}0\\2\Gamma_m^+\end{pmatrix}^T = \begin{pmatrix}1\\1\end{pmatrix}^T \begin{pmatrix}0 & 0\\ 0 & 2\Gamma_m^+\end{pmatrix}$$

$$= \begin{pmatrix}1\\1\end{pmatrix}^T (\mathbb{1} - \sigma_z^m) \Gamma_m^+$$

$$= \langle \Gamma_m^+ \rangle - \langle \sigma_z^m \Gamma_m^+ \rangle - \langle \Gamma_m^- \rangle - \langle \sigma_z^m \Gamma_m^- \rangle$$

$$= \frac{1}{2} \langle \sigma_z^{m-1} + \sigma_z^{m+1} \rangle \tanh(2\beta\varepsilon) - \frac{1}{2} \langle \sigma_z^m + \sigma_z^m \rangle$$

$$= - \langle \sigma_z^m \rangle + \frac{1}{2} \left(\langle \sigma_z^{m-1} \rangle + \langle \sigma_z^{m+1} \rangle \right) \tanh(2\beta\varepsilon)$$

Coarsening in the Ising model

- having access to the time depence of observables of the Ising model allows to consider non-equilibrium situations
- interesting is for instance to understand the evolution of a paramagnet after the temperature is suddenly changed to below T_c (this is called a quench)
- the stationary state should be magnetized, but how this state is assumed from a paramagnetic initial condition is surprisingly interesting
- the phenomenon occurring here is called coarsening
- this means that after the quench domains of locally uniform magnetisation are grown in a self-similar way
- the typical size of the magnetic domains, L, follows a power-law as a function of time, i.e $L \propto t^n$, with the power n being dependent on the considered dynamics e.g. Glauber dynamics

- we study this phenomenon using the correlation $C(|i-j|,t) = \langle \sigma_z^i \sigma_z^j \rangle(t)$
- this function follows the equation of motion

$$r \neq 0: \quad \partial_t C(r,t) = C(r+1,t) - 2C(r,t) + C(r-1,t)$$

$$r = 0: \quad C(0,t) = 1 \quad \text{for all times}$$

- in order to solve this equation we consider the continuum limit, i.e. we assume, that the separation r between spins is a continuous variable
- we can then approximate:

$$C(r\pm 1,t) \approx C(r,t) \pm \frac{\partial}{\partial r} C(r,t) + \frac{1}{2}\frac{\partial^2}{\partial r^2} C(r,t)$$

$$\hookrightarrow \partial_t C(r,t) = \partial_r^2 C(r,t)$$

- this is the diffusion equation, which indeed has a so-called scaling solution, in which time and space are connected via a power law: $C(r,t) = f(\underbrace{r t^{-1/2}}_{x})$

- inserting the scaling ansatz into the differential equation leads to

$$\partial_x^2 f(x) = -\frac{x}{2}\partial_x f(x)$$

- integrating with the boundary conditions $f(0) = 1$ and $f(\infty) = 0$ leads to

$$C(r,t) = \operatorname{erfc}\left(\frac{r}{2t^{1/2}}\right) \; ; \; \overbrace{\operatorname{erfc}(x)}^{\text{complementary error function}} = 1 - \frac{2}{\sqrt{\pi}}\int_0^x d\tau\, e^{-\tau^2}$$

- this is the time dependence of the correlation function in the domain growth / coarsening regime
- under the Glauber dynamics the typical domain size L therefore follows

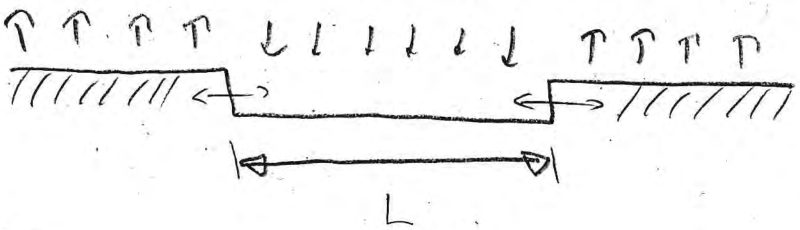
$$L \propto t^{1/2}$$

- the same result can actually be found with the following simple considerations:
- at $T=0$ only the following two processes have a non-zero rate

domain wall diffusion

domain wall annihilation

- the borders (walls) of a domain of length L

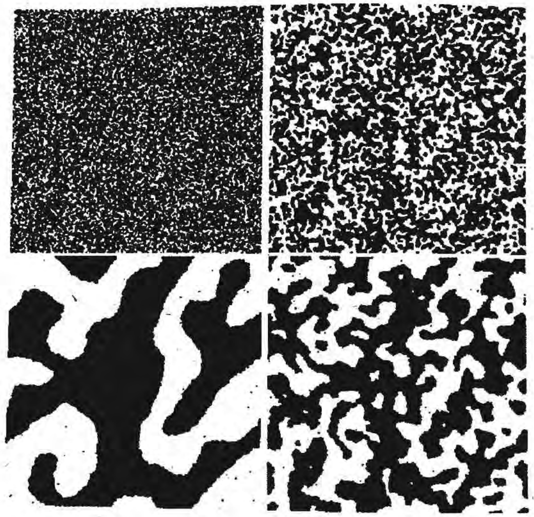


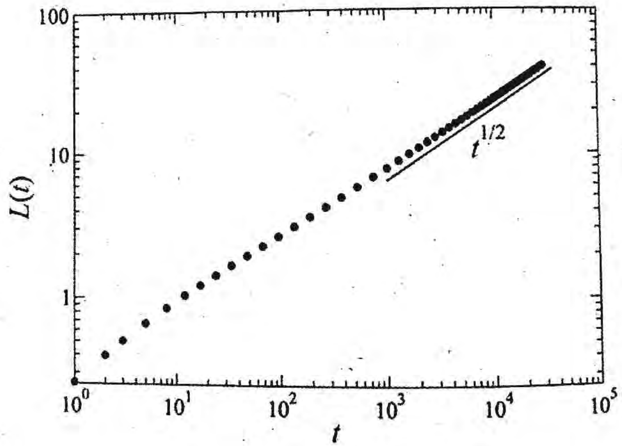
perform a random walk, and in order for both walls to meet and annihilate on average L^2 time steps (spin flips) are required

- therefore: $t_{\text{annihilation}} \propto L^2$, which confirms the previously found scaling
- this result is a direct consequence of the fact that at zero temperature the Glauber dynamics leads to domain wall diffusion
- So one would expect that a different type of dynamics could lead to different scaling behaviour

Glauber dynamics

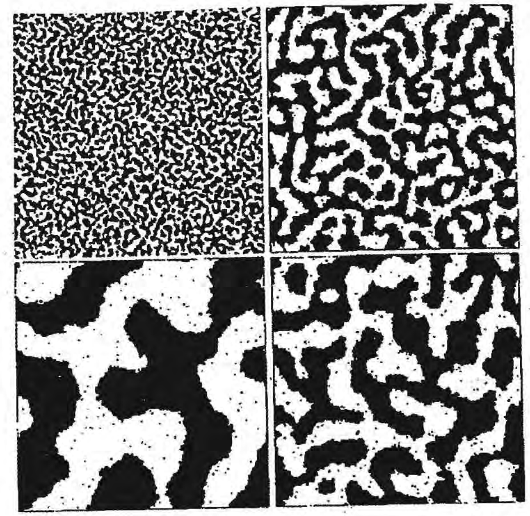
- 1000 x 1000 sites
- Quench from infinite T to $T=0.661\,T_c$
- $T=10, 10^2, 10^3, 10^4$

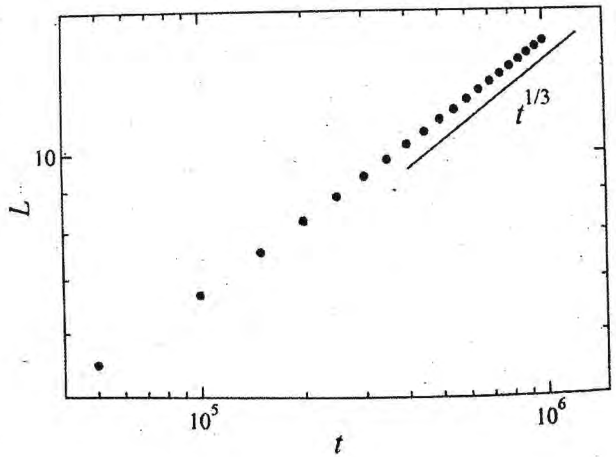




Kawasaki dynamics

- 256 x 256 sites
- Quench from infinite T to $T=0.661\,T_c$
- $T=10^2, 10^4, 10^5, 10^6$





- this is indeed the case, and we will study this using the so-called <u>Kawasaki spin-exchange dynamics</u>
- this dynamics conserves the magnetisation, i.e. the number of up and down spins is not changed under the dynamics
- the dynamical rules are as follows:

energy change

$\downarrow \downarrow \downarrow \uparrow \downarrow \downarrow \downarrow$ particle diffusion, $\Delta E = 0$

$\uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \uparrow$ hole diffusion, $\Delta E = 0$

$\uparrow \uparrow \uparrow \downarrow \uparrow \downarrow \downarrow$ particle attachment, $\Delta E < 0$

$\uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow$ particle detachment, $\Delta E > 0$

- let us now consider the dynamics of a domain configuration of the following form:

$$\underbrace{\uparrow \uparrow \uparrow \uparrow \uparrow}_{\sim L} \; \underbrace{\downarrow \downarrow \downarrow \downarrow \downarrow}_{L} \; \underbrace{\uparrow \uparrow \uparrow \uparrow}_{\sim L}$$

- the first difference to the Glauber dynamics is that at $T = 0$ nothing can move
- i.e. we need a finite temperature, so that the first spin can detach: $\uparrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \rightarrow \uparrow \uparrow \uparrow \downarrow \uparrow \downarrow$

- this is happening on a time scale $\tau_0 \sim e^{2\beta\varepsilon}$, since the rate is $\sim e^{-2\beta\varepsilon}$
- suppose that such detachment is happening, then an up spin has to move by L sites in order to travel from one to the other domain of up-spins
- this happens with probability $p(L)$, and thus the time for one spin moving from one $\uparrow\uparrow$-domain to the other is

$$\tau_0 \approx e^{2\beta\varepsilon}/p(L)$$

- to estimate the time at which one $\uparrow\uparrow$-domain has completely moved over to the other $\uparrow\uparrow$-domain, one needs to realise that in fact the $\downarrow\downarrow$-domain needs to move by L sites in order for that to happen
- this is a random walk which requires on average L^2 steps
- hence the timescale for the merging of the $\uparrow\uparrow$-domains is $t(L) \approx e^{\beta\varepsilon_0} \dfrac{L^2}{p(L)}$

- the probability $p(L)$ can be calculated as follows:

$$p(L) = p(L-1) \times \frac{1}{2}$$ = (probability of hopping $L-1$ sites) × (probability to hop to the final site)

$$+ p(L-1) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2}$$ = (prob. of hopping $L-1$ sites) × (prob of not hopping to final site) × (prob. of not hopping back to the other domain) × (prob. of hopping to final site)

$$+ p(L-1) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2} \times (1-p(L-1)) \times \frac{1}{2}$$
$$+ \dots$$
$$= \frac{p(L-1)}{2} \sum_{n=0}^{\infty} \left[\frac{1-p(L-1)}{2}\right]^n = \frac{p(L-1)}{1+p(L-1)}$$

↳ $p(L) = \frac{p(L-1)}{1+p(L-1)} \rightarrow p(L) = \frac{1}{L}$

- hence, the time scale for the merging of the ↑↑-domains is

$$t(L) \approx e^{\beta E_0} L^3 \rightarrow L \sim t^{1/3}$$

- the power law for the scaling regime of the coarsening dynamics is different to the Glauber dynamics

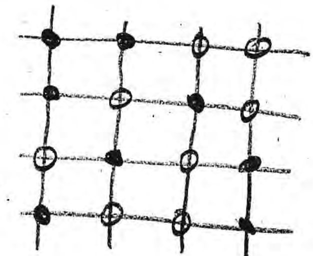
- This difference in the scaling behaviour is in fact a consequence of the conservation law of the Kawasaki dynamics

Out-of-equilibrium processes and phase transitions

- we will now consider phase transitions in many-body systems which cannot be described within the framework of equilibrium statistical mechanics
- for these out-of-equilibrium processes we cannot formulate a canonical partition function
- they are described merely through their dynamics, which may be formulated by a Markovian master equation
- paradigmatic examples are given by dynamical processes that feature an absorbing state, for instance some cellular automata
- an absorbing state is a microstate that can be entered dynamically, but which cannot be left anymore (this violates detailed balance)

- an example is given by the <u>contact process</u>

- it is defined on a d-dimensional square lattice, whose sites are labelled by k
- each site can either be empty ($S_k = 0$; healthy) or occupied ($S_k = 1$; infected)
- the state of the lattice is updated, i.e. propagated in time, via the following rules:



∘ healthy
• infected

– probability for going from infected to healthy

$$w(1 \to 0) = \Gamma \qquad \bullet \longrightarrow \circ$$

↳ an infected site can spontaneously heal

– probability for going from healthy to infected

$$w(0 \to 1) = \frac{\lambda}{2d} \times (\text{number of infected neighbors})$$

$$\bullet\,\circ \longrightarrow \bullet\,\bullet$$

↳ a site can only be infected if at least one of its neighbors is infected

→ the state in which all sites are healthy is absorbing, i.e. once it is reached one cannot escape

- we can cast this dynamics into a master equation by introducing the operators

$n_k = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\sigma_z^k + 1}{2}$, which projects on the infected state of site k

- using furthermore the spin raising and lowering operators, $\sigma_k^{\pm}$, we find for the contact process in 1 dimension the following equation:

$$\partial_t |p\rangle = \overbrace{\sum_k \underbrace{r\left[\sigma_k^- - n_k\right]}_{\text{spontaneous healing}} + \underbrace{\frac{\lambda}{2}\left(n_{k-1}+n_{k+1}\right)\left[\sigma_k^+ - (1-n_k)\right]}_{\text{infection due to infected neighbours}}}^{W \text{ (dynamical operator)}} |p\rangle$$

- we can now calculate the time evolution of the local density of infected sites

$$\partial_t \langle n_m \rangle = \langle \mathbb{1} | n_m \partial_t | p \rangle = -r \langle n_m \rangle + \frac{\lambda}{2} \langle (n_{m-1} + n_{m+1})(1-n_m) \rangle$$

- this is not a closed equation, because the right-hand-side depends on the correlation functions $\langle n_{m-1} n_m \rangle$, which themselves are subjects to an equation of motion

$$\partial_t \langle n_{m-1} n_m \rangle = \langle \mathbb{1} | n_{m-1} n_m W | p \rangle \propto \langle n_{m-1} n_m n_{m+1} \rangle + \ldots$$

- this hierarchy of coupled equations never closes

- for an approximate solution we employ a mean field approximation:

$\langle n_{m-1} n_m \rangle \approx \langle n_{m-1} \rangle \langle n_m \rangle$ multi-site correlations are neglected

$\langle n_{m-1} \rangle \approx \langle n_m \rangle = \rho$ the density of infected sites is assumed to be homogeneous

- this leads to the following mean field equation: $\partial_t \rho = \lambda \rho (1-\rho) - r\rho = (\lambda - r)\rho - \lambda \rho^2$

- realising, that $\dfrac{d\rho}{\lambda\rho\left(\frac{\lambda-r}{\lambda} - \rho\right)} = \dfrac{d\rho}{(\lambda-r)\,\rho} + \dfrac{d\rho}{(\lambda-r)\left[\frac{\lambda-r}{\lambda} - \rho\right]}$

the mean field equation can be integrated

- using the initial condition $\rho(0) = 1$ (initially the lattice is filled with infected sites), we find the solution

$$\rho(t) = \frac{\lambda - r}{\lambda - e^{-(\lambda-r)t}\, r}$$

density of infected sites

$$(\lambda-r)t = c + \log \rho - \log\left(\frac{\lambda-r}{\lambda} - \rho\right)$$

$$= c + \log \frac{\rho}{\frac{\lambda-r}{\lambda} - \rho}$$

$$\hookrightarrow c' e^{(\lambda-r)t} = \frac{\rho}{\frac{\lambda-r}{\lambda} - \rho}$$

$$t = 0 \rightarrow \rho = 1$$

$$\hookrightarrow c' = \frac{1}{\frac{\lambda-r}{\lambda} - 1} \rightarrow c' = \frac{1}{-\frac{r}{\lambda}} = -\frac{\lambda}{r}$$

$$\hookrightarrow -\frac{\lambda}{r} e^{(\lambda-r)t}\left(\frac{\lambda-r}{\lambda} - \rho\right) = \rho$$

$$-\frac{\lambda-r}{r} e^{(\lambda-r)t} + \frac{\lambda}{r} \rho e^{(\lambda-r)t} = \rho$$

$$\frac{\lambda-r}{r} e^{(\lambda-r)t} = \rho\left(\frac{\lambda}{r} e^{(\lambda-r)t} - 1\right)$$

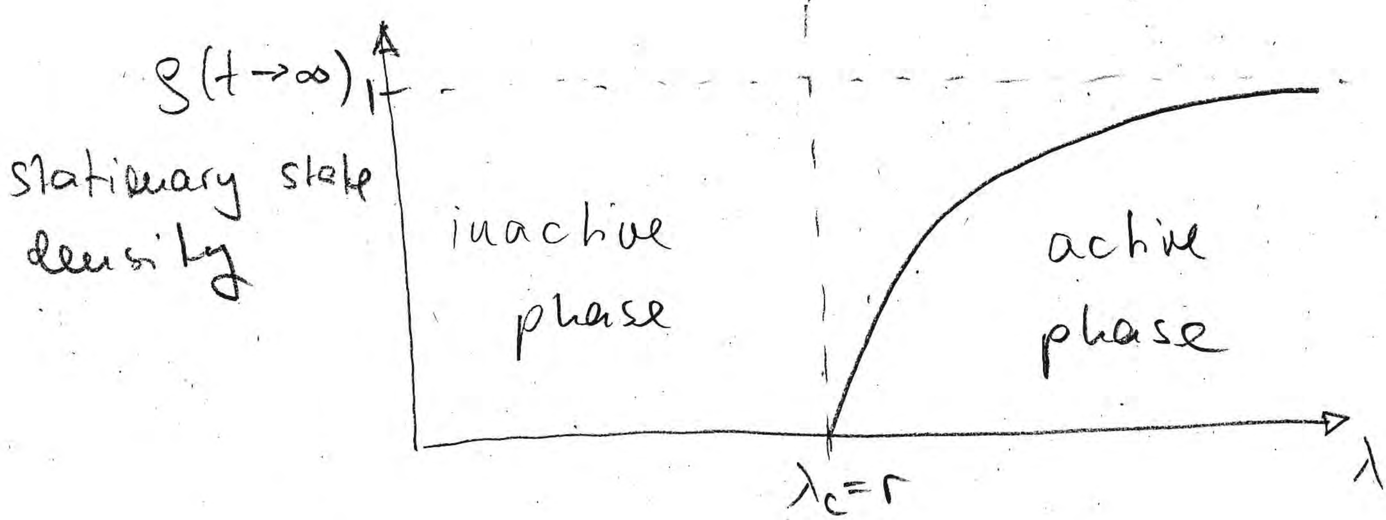
$$\hookrightarrow \rho = \frac{\lambda-r}{r} \frac{e^{(\lambda-r)t}}{\frac{\lambda}{r} e^{(\lambda-r)t} - 1} = \frac{\lambda - r}{\lambda - r e^{-(\lambda-r)t}}$$

- if the infection rate λ is smaller than the recovery rate, we find that the density of infected sites tends to zero: $\rho(t \to \infty) = 0 \quad , \lambda < r$

- Conversely, when $\lambda > r$, we find that

$$\rho(t \to \infty) = \frac{\lambda - r}{\lambda}$$

- apparently, $\lambda_c = r$ marks a critical value of the infection rate, below which the system goes to the (inactive) absorbing state
- above λ_c the system is in the so-called active phase in which it maintains a finite density of infected sites



- the transition between the inactive and active phase is continuous
- it can be characterised by a set of critical exponents, which define the so-called <u>directed percolation universality</u> class
- one exponent is obtained by studying the stationary state density ρ, near stationarity

$$\rho(t\to\infty) = \frac{1}{\lambda}(\lambda - r) = \frac{1}{\lambda}(\lambda-\lambda_c) \propto (\lambda-\lambda_c)^{\beta}$$

$\hookrightarrow \beta = 1$

- another exponent can be found by investigating the time dependence at criticality:

$$\lim_{\lambda\to r} \rho(t) = \frac{1}{1+rt} \xrightarrow{rt \gg 1} t^{-\delta}$$

$\hookrightarrow \delta = 1$

- furthermore, we can identify an exponent by analysing the correlation time in the inactive phase

$$\rho(t) \overset{rt \gg 1}{\approx} (r-\lambda)\exp\left[-\frac{t}{\xi_{\parallel}}\right]$$, with $\xi_{\parallel}$ being the correlation time

$\hookrightarrow \xi_{\parallel} \sim (\lambda-\lambda_c)^{-\nu_{\parallel}}$ with $\nu_{\parallel} = 1$

- the exponents we have obtained so far are mean field exponents
- the actual exponents have to be calculated numerically
- just like for the Ising model, they depend on dimensionality

	mean field	1d	2d	3d
β	1	0.276	0.584	0.81
δ	1	0.159	0.451	0.73
$\nu_{\parallel}$	1	1.734	1.295	1.11
$\nu_{\perp}$	1/2	1.097	0.451	0.73

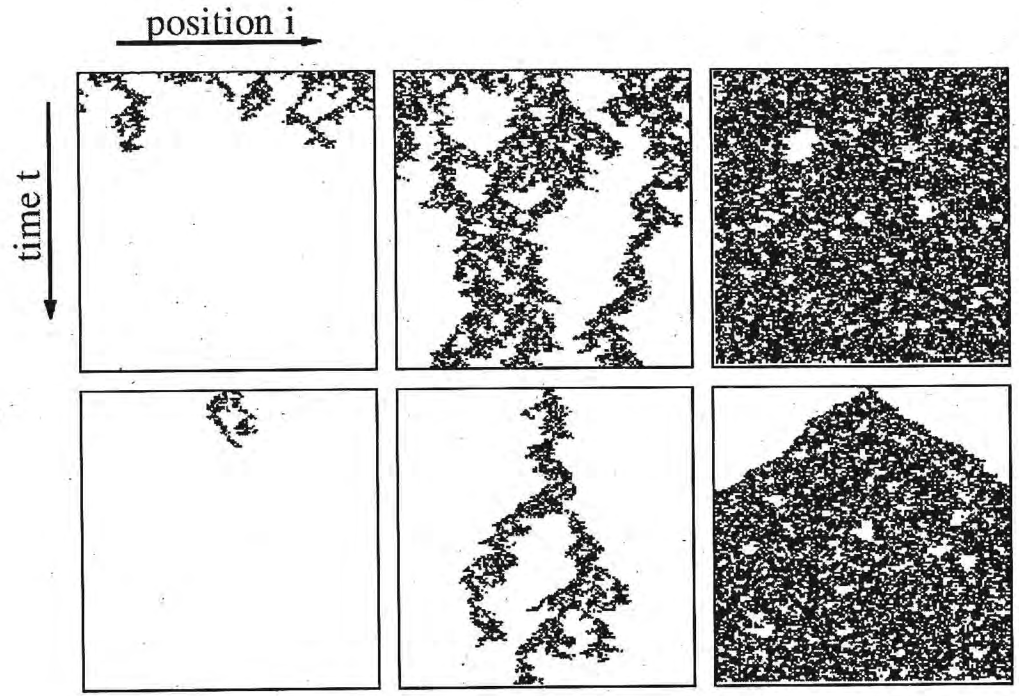
correlation length in space

- the actual critical point in 1d is $\lambda_c = 3.298\,r$

- note, that in contrast to the Ising model there is a phase transition already in one dimension

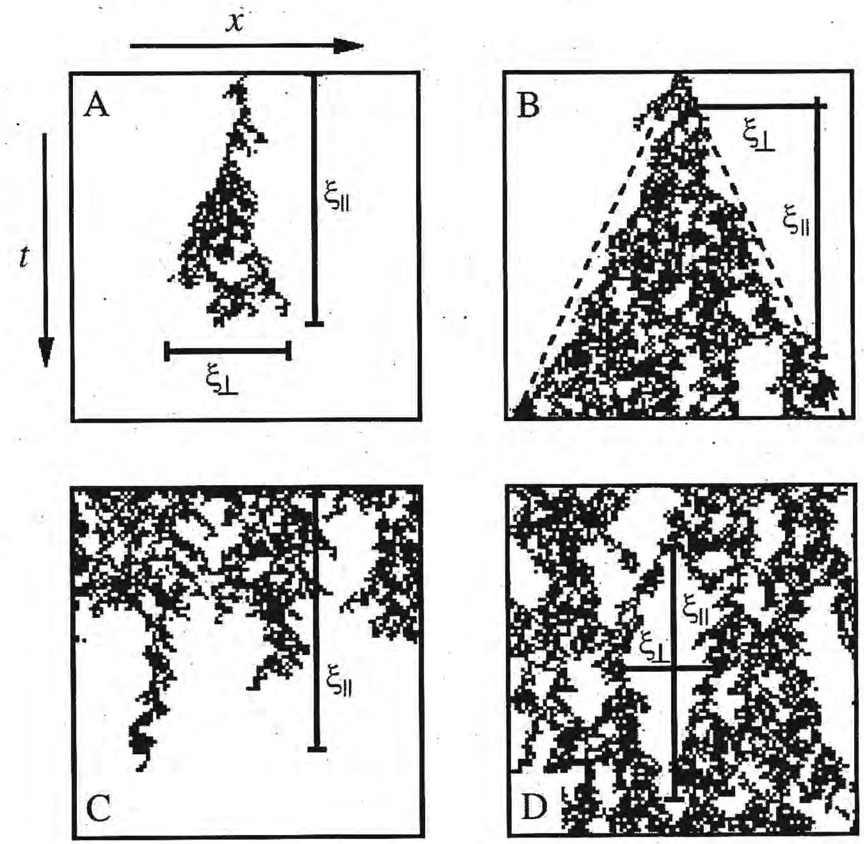
Phase transition in the contact process

- Inactive and active phase



$\lambda < \lambda_c$ $\lambda = \lambda_c$ $\lambda > \lambda_c$

- Correlation lengths

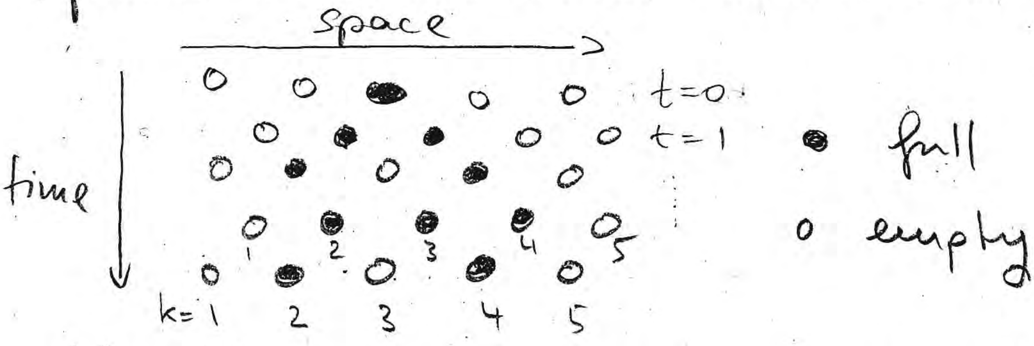


$\lambda < \lambda_c$ $\lambda > \lambda_c$

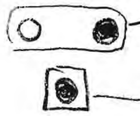
Domany-Kinzel cellular automata

- many basic models of nonequilibrium phase transitions can be formulated as dynamical processes of particles moving on a lattice
- cellular automata are a particular class:
  - each lattice site can at most be occupied by a single particle (exclusion)
  - the dynamical rules are local, i.e. state changes of a particle depend only on particles in the direct neighbourhood
  - the dynamics is Markovian, i.e. the configuration at time $t+1$ depends only on configuration at time t
- deterministic cellular automata were introduced at the beginning of the 20th century by John von Neumann
- Domany and Kinzel introduced stochastic (probabilistic) cellular automata in the 1980s, which serve as an important paradigm for non-equilibrium processes

- DK models are defined on a tilted square lattice whose sites are either empty or full

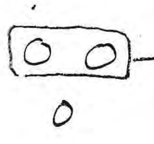


- the horizontal | vertical directions are space | time
- all sites of the lattice are initially empty, except for the first line, which contains the initial state
- the propagation in time proceeds line by line, where the line corresponding to time t is updated depending on the state of line $t-1$
- the update rules are


— configuration at $t-1$
— fill site at time t with probability p


— fill with probability p


— fill with probability q


— don't do anything if there are two empty sites at time t

- the DK models have (at least) one absorbing state, which is the empty state ○ ○ ○ ○ ○ ○
- therefore, it is not really surprising that there is an extremely close link to the contact process and the directed percolation universality class
- this can be seen by considering the evolution of the density of filled sites $\langle n_k^t \rangle$; $n_k^t = | \bullet \underset{k}{\times} \bullet |_t$
  ↳ the dynamical rules lead to the following equation:

$$\langle n_k^{t+1} \rangle = p \langle n_k^t (1-n_{k+1}^t) \rangle + p \langle (1-n_k^t)\, n_{k+1}^t \rangle + q \langle n_k^t n_{k+1}^t \rangle$$

- employing a mean field treatment as we have done already in case of the contact process, and denoting $\rho_t = \langle n_k^t \rangle = \langle n_{k+1}^t \rangle$, one finds for the density of filled sites the following difference equation:

$$\rho_{t+1} - \rho_t = 2p\,\rho_t (1-\rho_t) + q\,\rho_t^2 - \rho_t$$

- turning this into a differential equation, using $\rho_{t+1} - \rho_t \approx \partial_t \rho$ and rearranging the terms, yields

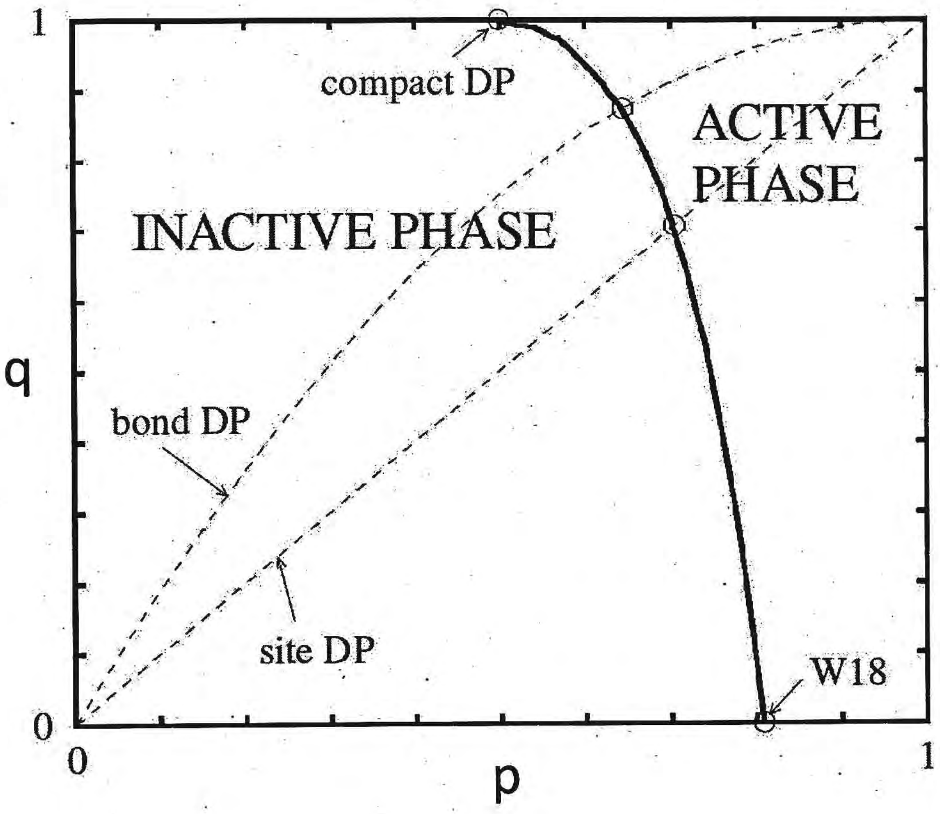
$$\partial_t \rho(t) = (2p-1)\,\rho(t) - (2p-q)\,\rho^2(t)$$

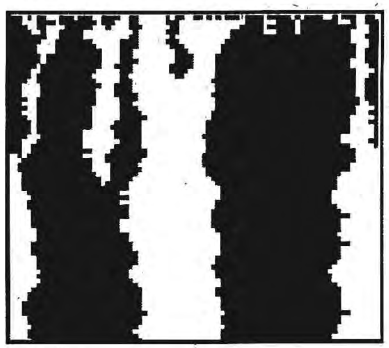
- this is precisely the same mean field equation that we obtained for the contact process
- in fact it turns out that also the DK cellular automata feature a phase transition between an absorbing state and an active phase which is in the directed percolation universality class, i.e. the critical exponents are the same
- <u>except</u>, when $q=1$!
- here the mean field equation becomes

$$\partial_t \rho(t) = (2p-1)\,\rho(t)\,[1-\rho(t)]$$ and

apparently both, the empty state ($\rho = 0$) and the completely filled state ($\rho = 1$) are stationary states of the dynamics

Phase diagram of the Domany-Kinzel cellular automaton



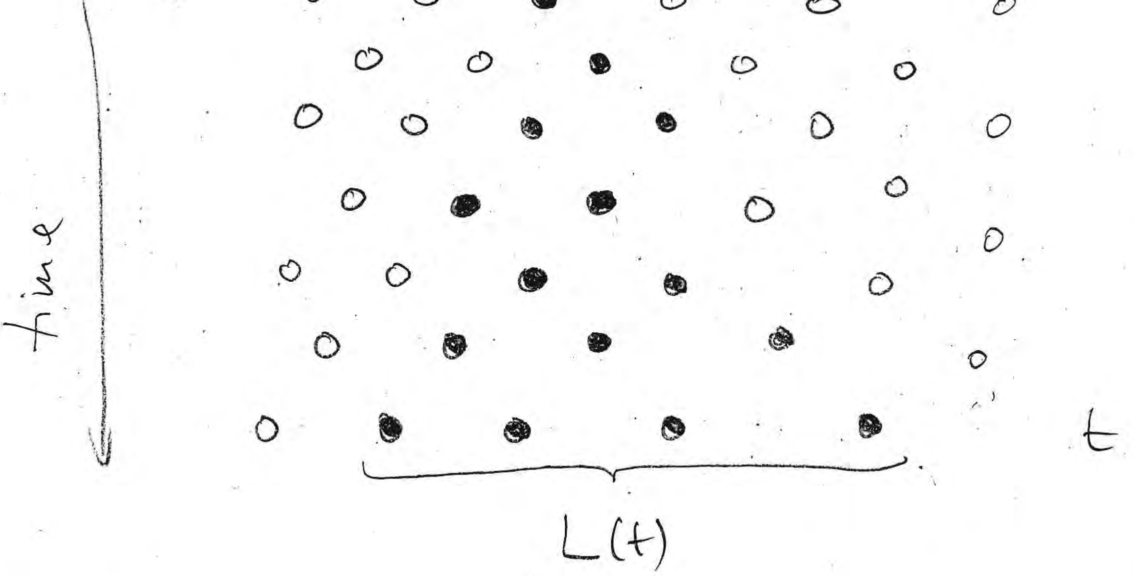


compact DP

bond DP

Wolfram rule 18

- this dynamics has a higher symmetry than the contact process because it is invariant under the exchange of healthy and infected sites $\bullet \leftrightarrow \circ$
- this is a so-called particle-hole symmetry, which not only leads to two absorbing states ($\circ\circ\circ\circ$ and $\bullet\bullet\bullet\bullet$) but results also in different universal behaviour near the transition between the active and the inactive phase
- the universality class in this case goes under the name <u>compact directed percolation</u>
- the name stems from the fact that the dynamics creates compact clusters, i.e. clusters of infected sites without holes



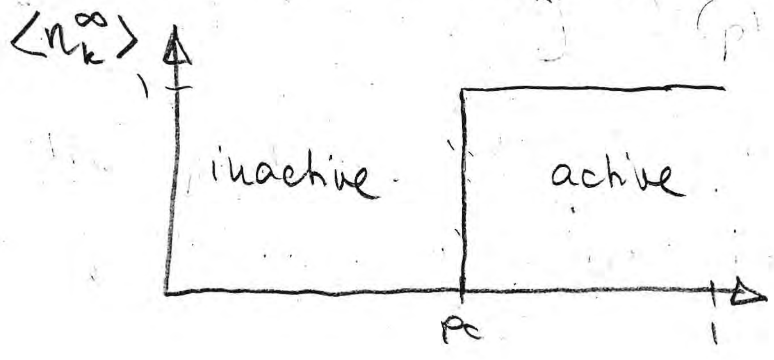
- the phase transition point can be directly inferred from the particle-hole symmetry
- we have

	● ● ●	● ○ ●	○ ● ●	○ ○ ●
with probability	1	p	p	0
and	● ● ○	● ○ ○	○ ● ○	○ ○ ○
with probability	0	1-p	1-p	1

- however, we can exchange hole and particles, such that for the critical value of p it must hold that: $p_c = 1 - p_c$

$$\hookrightarrow p_c = \frac{1}{2}$$

- below the critical point the stationary state is the empty one: ○ ○ ○ ○ ○ ○
- by symmetry, however, the stationary state must be the completely filled one: ● ● ● ● ●
- therefore, the stationary state density of occupied sites, $\langle n_k^\infty \rangle$, follows



- this behaviour is markedly different with respect to the contact process
  ↳ near the critical point the density of filled sites behaves as

$$\langle n_k^\infty \rangle \propto (p - p_c)^\beta \quad \text{with } \beta = 0$$

- this „critical exponent" is clearly different to that of the directed percolation universality class
- we can find another critical exponent by studying the survival probability $P(p)$ of a seed; $\circ\ \circ\ \circ\ \underbrace{\bullet}_{L(t)}\ \circ\ \circ\ \circ$, as a function of p
- in each time step the size $L(t)$ of the cluster of filled sites can either grow, shrink or remain constant:

$$L(t+1) = \begin{cases} L(t) + 1, & \text{with probability } p^2 \\ L(t), & \text{with probability } 2p(1-p) \\ L(t) - 1, & \text{with probability } (1-p)^2 \end{cases}$$

- hence, $L(t)$ performs an asymmetric random walk with a probability
$$r = \frac{p^2}{p^2 + (1-p)^2}$$
to move to the right and probability $1-r$ to move to the left (the probability for maintaining the length is not important here, as it merely changes the duration of an effective time step)
- in order to calculate $P(p)$ we need to compute the probability that $L(t=\infty) = \infty$, knowing that $L(0) = 1$ and that there is an absorbing barrier at $L=0$ (here the system enters the absorbing state 00000)
- this problem is actually known as the "Gambler's ruin": here $L(t)$ is the amount of Euros the gambler possesses and in each time step he/she can win or lose 1 Euro
- bankruptcy therefore corresponds to $L=0$, and the survival probability $P(p)$ is thus just the probability winning ω Euros with $\omega \to \infty$, starting with 1 Euro

- the probability of winning w Euros, starting from n Euros shall be denoted by R_n

↳ $R_0 = 0$, started with 0 Euros makes it impossible to win

$R_w = 1$, having w Euros wins

- the gambler starts with n Euros and wins the first bet with probability r
- he/she then has $n+1$ Euros and thus the probability to reach w Euros is R_{n+1}
- conversely, if he/she loses with probability $1-r$, he/she remains with $n-1$ Euros and the probability to win w Euros is R_{n-1}

↳ this leads to the recurrence relation

$$R_n = r R_{n+1} + (1-r) R_{n-1} \quad (0 < n < w)$$

with boundary conditions

$R_0 = 0$ and $R_w = 1$

- the equation is solved with the ansatz $R_n = x^n$
- this yields the so-called characteristic equation

$$r x^2 - x + (1-r) = 0$$

- its solutions are

$$x = \begin{cases} \frac{1-r}{r} \\ 1 \end{cases}$$

- the solution of the recurrence relation is thus $R_n = a \cdot \left(\frac{1-r}{r}\right)^n + b \cdot 1^n$, where a and b have to be determined through the boundary conditions

$\hookrightarrow$ $0 = a + b$
$1 = a\left(\frac{1-r}{r}\right)^\omega + b$ $\longrightarrow$ $a = \dfrac{1}{\left(\frac{1-r}{r}\right)^\omega - 1}$

$b = -a$

- substituting back, this yields

$$R_n = \frac{\left(\frac{1-r}{r}\right)^n - 1}{\left(\frac{1-r}{r}\right)^\omega - 1}$$

- we are now interested in the limit $\omega \to \infty$ (cluster grows to infinity) and $r > \frac{1}{2}$.

$\hookrightarrow$ $$\lim_{\omega \to \infty} R_n = -\left(\frac{1-r}{r}\right)^n + 1$$

- the survival probability we are after is then given by R_1

$\hookrightarrow$ $$P(p) = \lim_{\omega \to \infty} R_1 = 1 - \left(\frac{1-r}{r}\right)$$
$$= \frac{2}{p^2}\left(p - \frac{1}{2}\right)$$

- close to criticality, i.e. $p = p_c + \varepsilon$, we thus find the scaling

$$P(p) \propto (p - p_c)^{\beta'} \quad \text{with } \beta' = 1$$

- the β'-exponent can also be determined for processes in the directed percolation universality class
- here $\beta = \beta'$, which is the consequence of the so-called rapidity reversal symmetry

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- for compact directed percolation, our exact solution shows that $\beta \neq \beta'$, and thus we find further confirmation that this universality class is different to directed percolation