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

order parameter

- 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

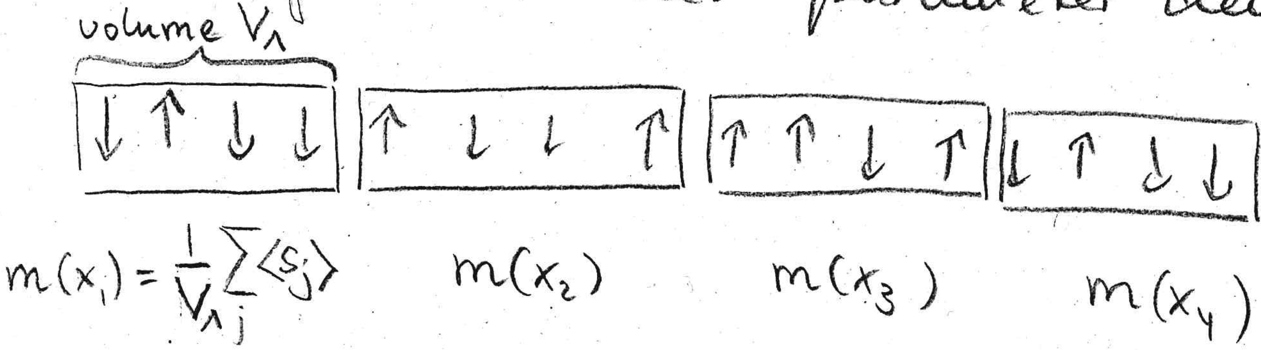
$$\mathcal{H}(\{\vec{S}_i\}) = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

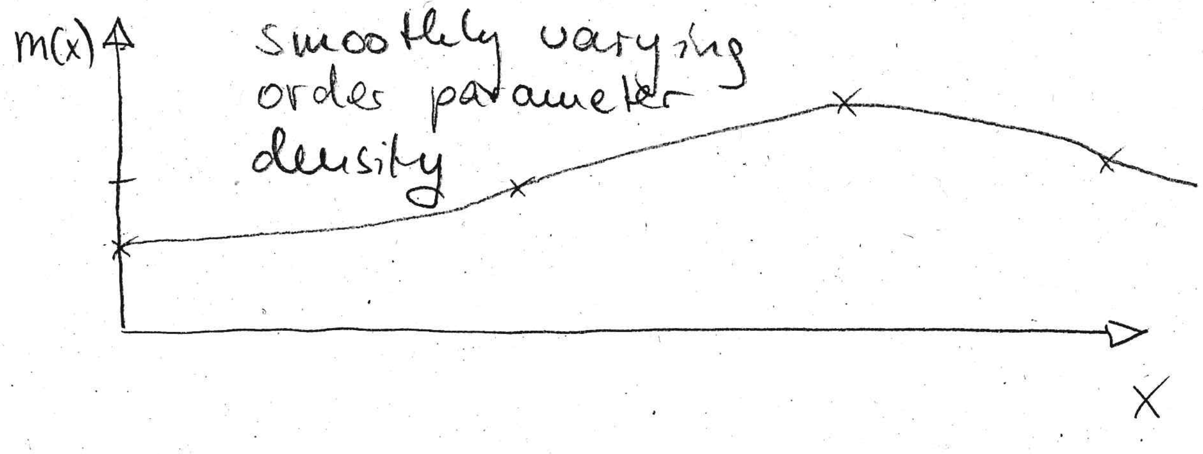
the order parameter is the magnetisation vector:

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

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





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

Hamiltonian

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

sum over all spin configurations

sum over all possible values of the local magnetisation density

sum over all microscopic configurations leading to a magnetisation density $m(x_i)$

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

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 $\tau = \frac{1}{1+t} \approx 1 - t + \dots$)

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

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

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

↳ 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

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

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

- 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:

$$\mathcal{L} = \sum_{n=0}^{\infty} a_n([K])\, \eta^n$$

numerical coefficients

coupling constants (H, J, T)

(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 $\eta \to -\eta$

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

$\frac{T-T_c}{T}$

- we write now $a_2 = a_2^0 + t\, a_2' + \dots$

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

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 $a_2 = \underbrace{a_2^0}_{=0} + t a_2'$

- 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

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

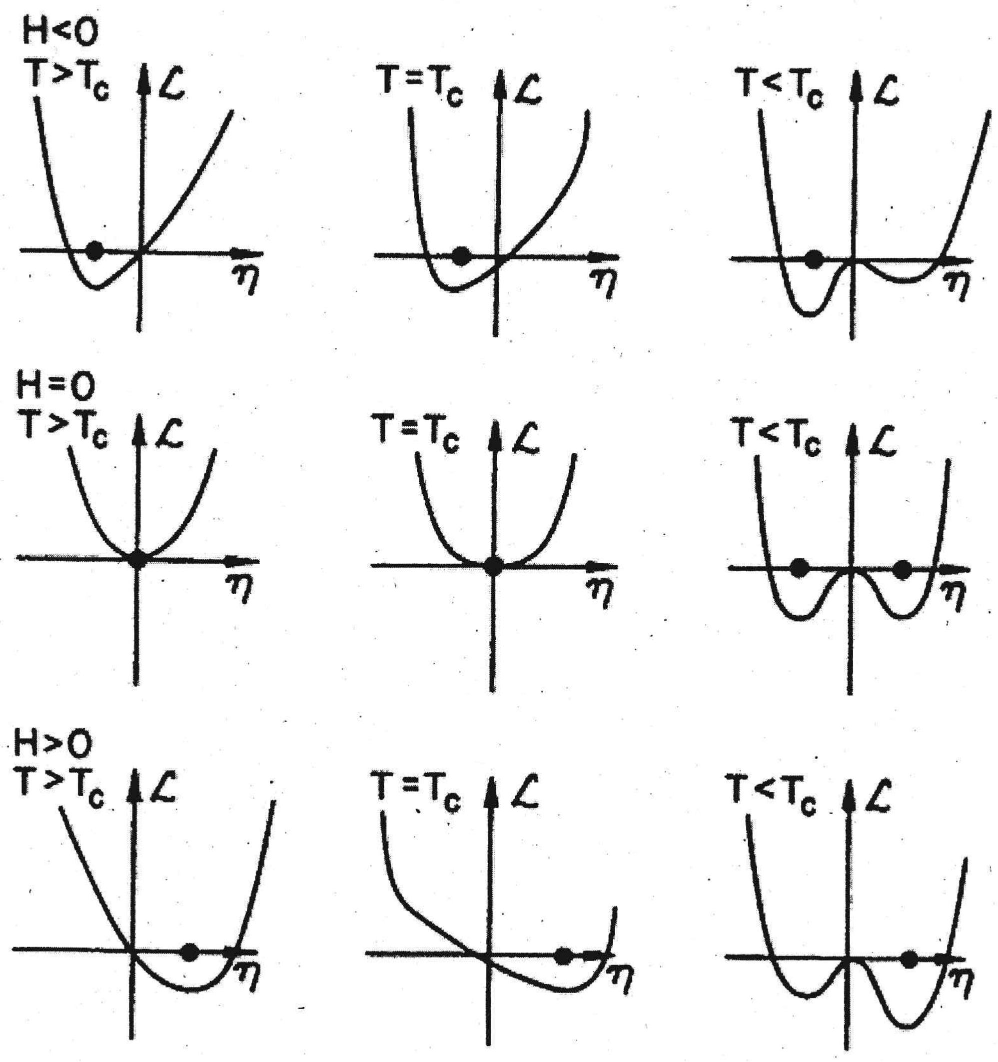


Figure 5.1 The Landau free energy density for various values of T and H. The • indicates the value of η at which $\mathcal{L}$ achieves its global minimum. The right-most column of graphs depicts the first order transition, which occurs for $T < T_c$ as H is varied from a negative to a positive value. 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 $\mathcal{L}_{min} = -\frac{1}{2}\frac{a^2t^2}{b}$, 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 $\eta \propto H^{1/\delta} \quad \rightarrow \quad \delta = 3$
- 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

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

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

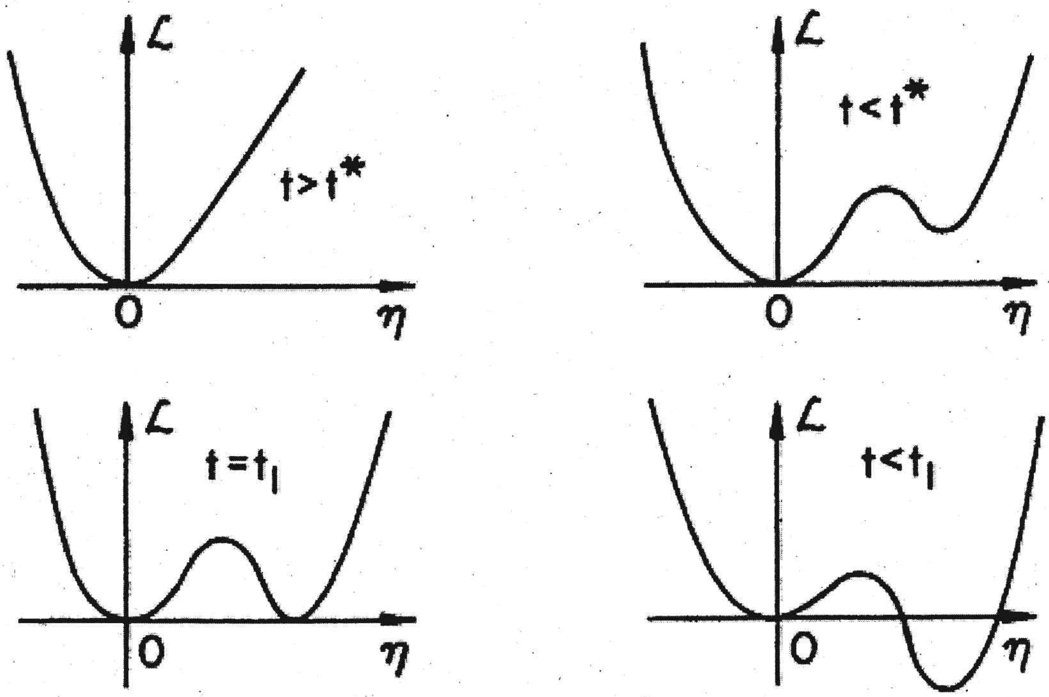


Figure 5.2 $\mathcal{L}$ as a function of η for various temperatures, showing the Landau theory description of a first order transition.

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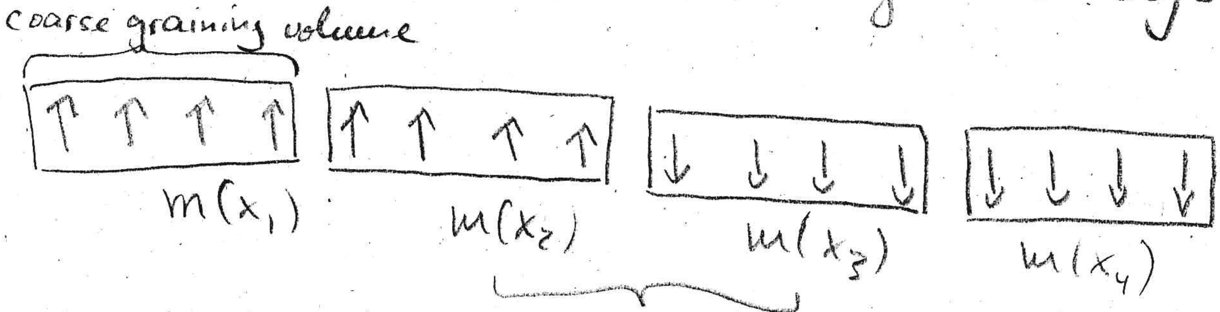
- when t is lowered below t_1, $\mathcal{L}$ is minimised by η_2 and the order parameter jumps discontinuously from zero to η_1
- this is a first order phase transition
- note, that Landau theory is not strictly valid at such a transition, because the order parameter does not become arbitrarily small

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

$$L = \underbrace{\int d^d \vec{r}}_{\text{integration over } d\text{-dimension space}} \left[\mathcal{L}(\{\eta(\vec{r})\}) + \frac{1}{2} \gamma \underbrace{\left(\nabla \eta(\vec{r}) \right)}_{\text{gradient of the order parameter density}}^2 \right]$$

previously considered Landau free energy density

positive constant

- 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

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

- 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

$$\int d^d\vec{r}\, e^{i(\vec{k}-\vec{k}')\vec{r}} = V\delta_{\vec{k}\vec{k}'}$$ ← 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

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

- (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, wich 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

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

$\hookrightarrow$ $\dfrac{\delta}{\delta\eta(\vec{r})} \displaystyle\int d^d\vec{r}'\, \eta(\vec{r}') = 1$; $\dfrac{\delta}{\delta\eta(\vec{r}')}\eta(\vec{r}) = \delta(\vec{r}-\vec{r}')$

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

- 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 $\chi(\vec{r},\vec{r}') = \chi(\vec{r}-\vec{r}')$ und $G(\vec{r},\vec{r}') = G(\vec{r}-\vec{r}')$
- 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

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

- 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

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

- 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:

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

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

$$\overset{!}{=} 0$$

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

- 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, $K_n(\varrho)$

exponentially decaying correlations in 1d

$$\hookrightarrow \frac{1}{g}\,\mathcal{G}(\varrho) = \begin{cases} e^{-\varrho} & , d=1 \\ \frac{1}{(2\pi)^{d/2}}\,\varrho^{-\frac{d-2}{2}}\,K_{\frac{d-2}{2}}(\varrho), & d \geq 2 \end{cases}$$

- the Bessel functions have the following asymptotic properties:

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

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

- we thus obtain away from criticality, where $r \gg \xi$ ($\varrho \gg 1$) 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

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

- <u>additional remarks:</u>
  - 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 the <u>Ginzburg criterion</u>

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

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

- 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

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

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

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 $\vec{v}^{(i)}$

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

$\tilde{\lambda}_i$ ↳ eigenvalues

↳ normal coordinates

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

- reparametersing $\frac{1}{\lambda_i^2} = \beta \tilde{\lambda}_i$, 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 $Z = e^{-\beta G}$

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

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

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

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

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

- 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:

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

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

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

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

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

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

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

(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

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

- 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

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

- 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 Josephson scaling law

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

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

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

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

- 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 $\chi_T = \beta \int d^d\vec{r}\; G(\vec{r})$

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

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

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

- the final relation we obtain from $\eta = -\left.\frac{\partial f}{\partial H}\right|_{H=0}$

- 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: $g(x) = ax^c$; $g(bx) = b^c a x^c \to g(x) = b^{-c} g(bx)$)

- 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 $r \to b^{-1} r$
- 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 $\chi_T \sim \int d^d\vec{r}\, G(r,t)$ 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

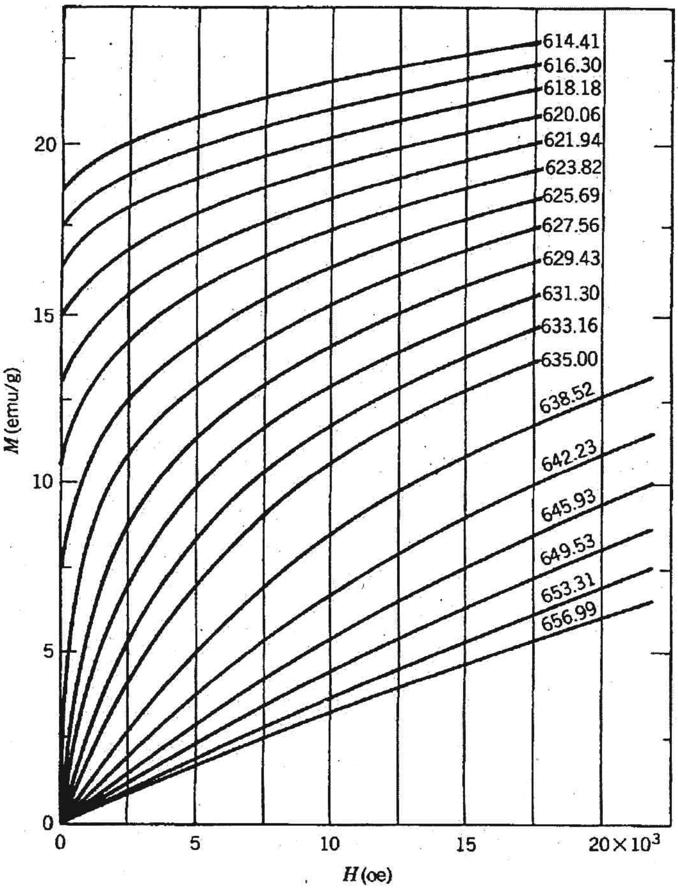
- hence $\eta \sim t^{\beta} \underbrace{S(|t|^{-\beta\delta} H)}_{\text{scaling function}}$

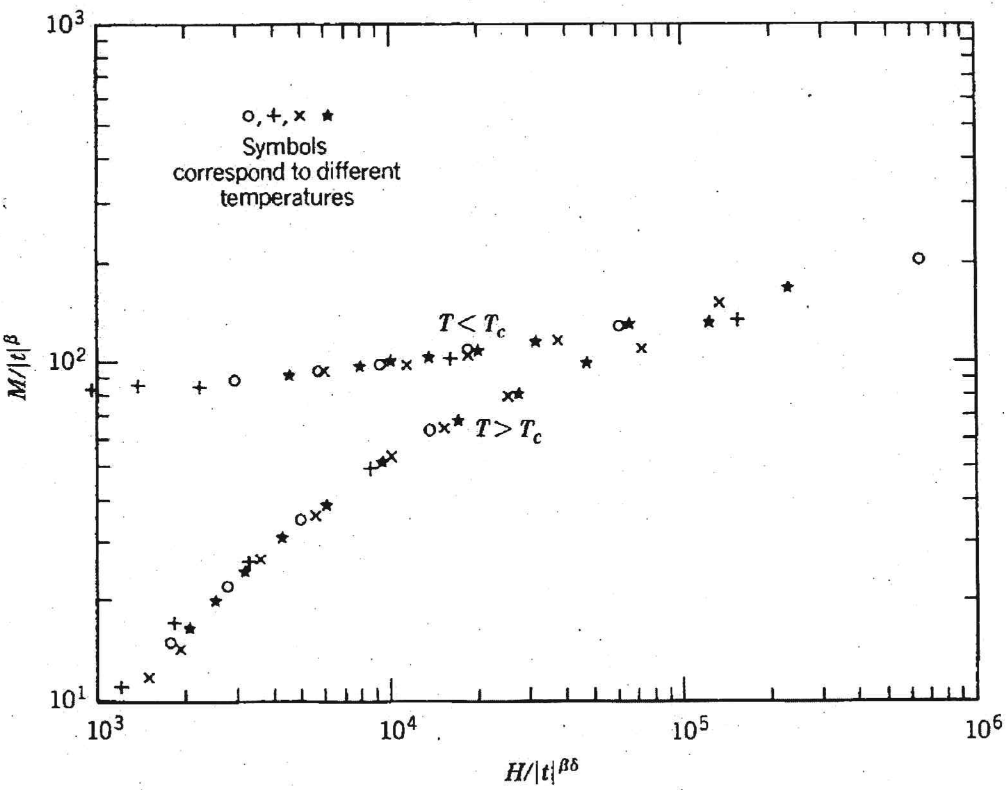
- this expression shows that the magnetisation density follows a universal behaviour near the phase transition point
- the scaling function S is typically different below and above T_c
- this result implies that when plotting $\eta|t|^{-\beta}$ as a function of $|t|^{-\beta\delta} H$ the results should 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 $[\beta\gamma] = \ell^0$, one has

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

ℓ^{d_η} ← 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 $G(\vec{r},\vec{r}')=\frac{1}{k_BT}\{\langle\eta(\vec{r})\eta(\vec{r}')\rangle-\langle\eta(\vec{r})\rangle\langle\eta(\vec{r}')\rangle\}$ 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 cut-off $\Lambda\sim\frac{1}{a}$
(wave number)
- 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

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

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

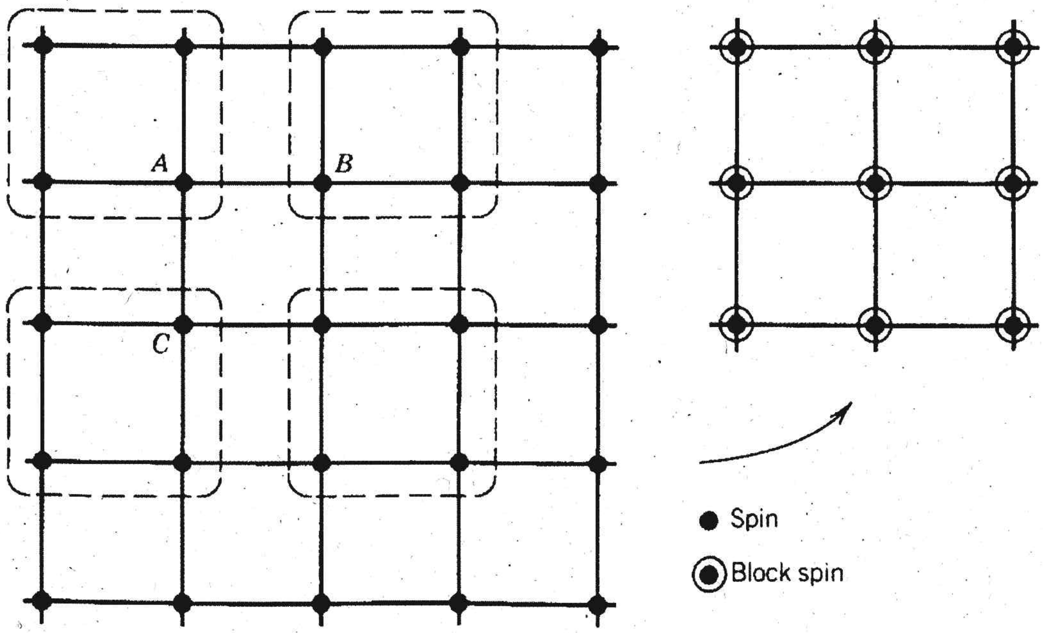


Fig. 18.1 Block-spin transformation: averaging the spins in a block, and then rescaling the lattice to the original size. In more than one dimension, the indirect interaction between B and C gives rise to next-to-nearest-neighbor interactions of the block spins.

Kerson Huang
Statistical Physics
John Wiley and Sons (1987)

- 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

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

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

  $\hookrightarrow$ $\xi_\ell = \frac{\xi_1}{\ell}$

- 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

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

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)

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

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

← 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. $\Delta = \beta\delta$

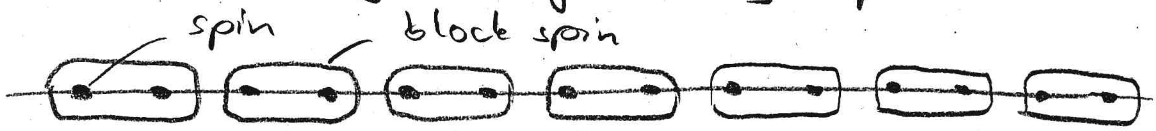
Block spin transformation in the one-dimensional Ising model

- 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

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

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

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

- 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.

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

- 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

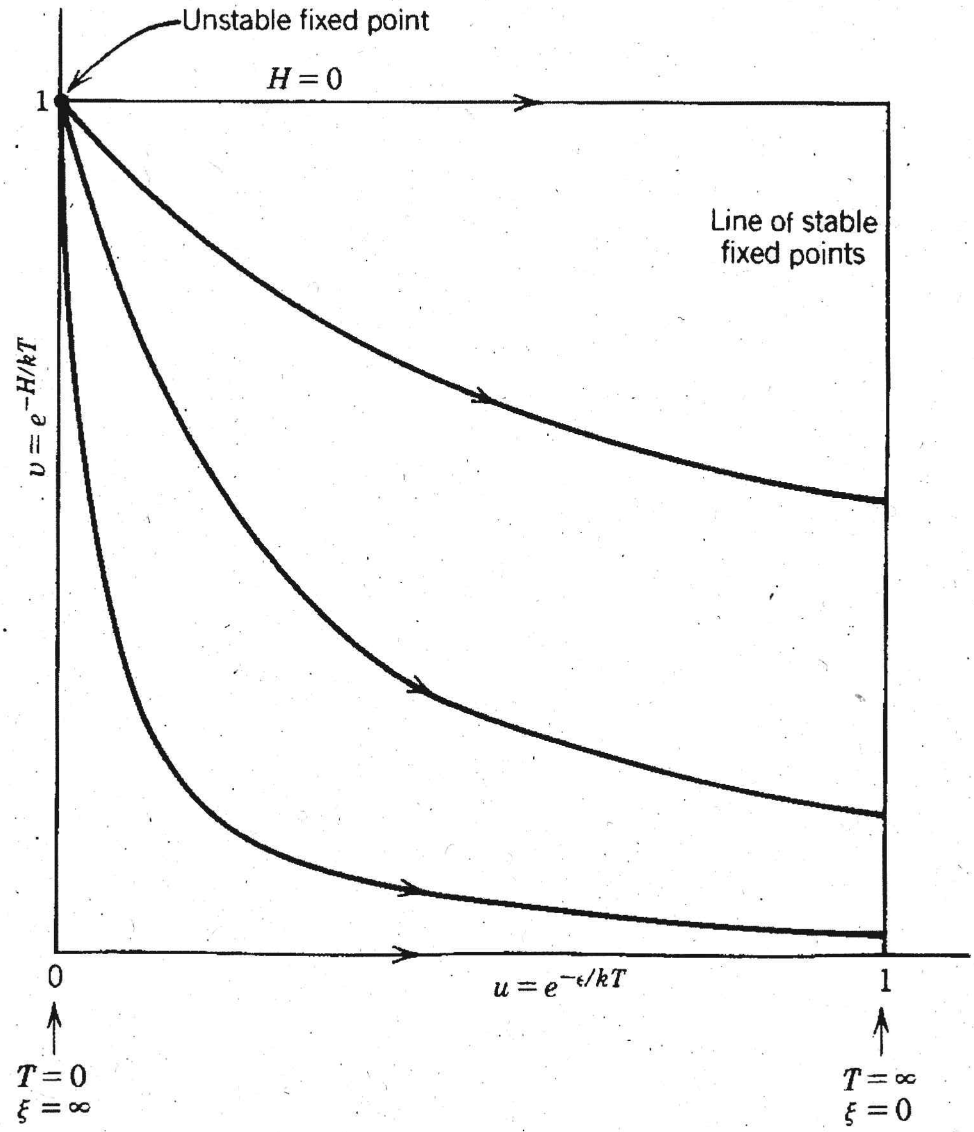


Fig. 18.3 Flow diagram of one-dimensional Ising model, showing how the coupling constant ϵ and the external field H change under successive block-spin transformations.

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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

$$\mathcal{H} = K_1 \sum_i s_i + K_2 \sum_{\substack{\langle ij\rangle \\ \text{nearest} \\ \text{neighbours}}} s_i s_j + K_3 \sum_{\substack{\langle\langle ij\rangle\rangle \\ \text{next-nearest} \\ \text{neighbours}}} s_i s_j + K_4 \sum_{\langle ijk\rangle} s_i s_j s_k + \ldots$$

- 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
  $\rightarrow$ 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

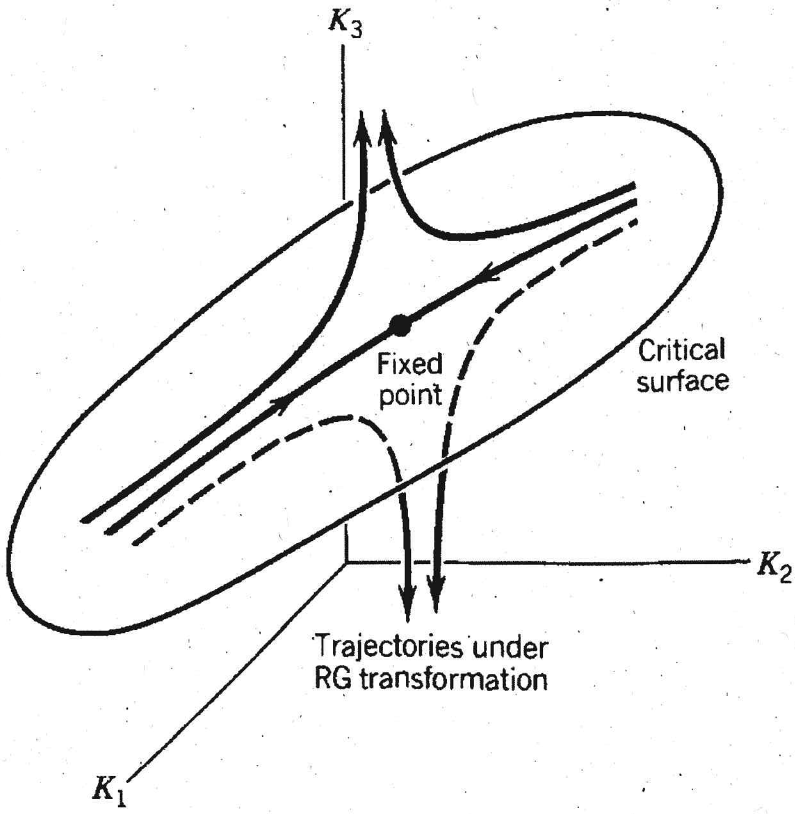

Fig. 18.4 The critical surface for a particular fixed point. It is a hypersurface in coupling-constant space obtained by setting all relevant variables to zero. Points on this surface correspond to systems in the same universality class, with the same critical exponents.

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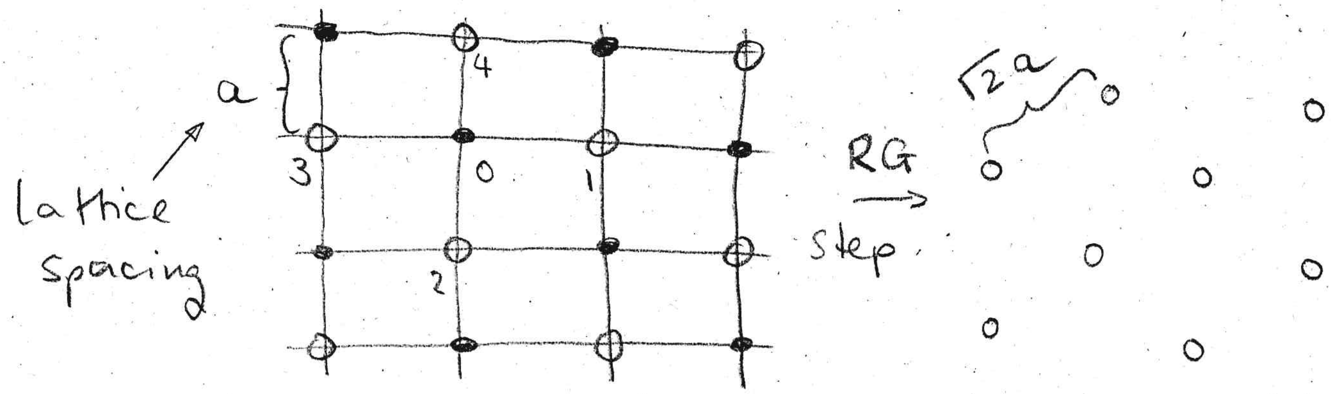
RG for the 2d Ising model on a square lattice

- 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

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

$\sum_{\{S_i\}}$: sum over all spins

$\sum_{\langle ij\rangle}$: sum over nearest neighbours

ε: Ising interaction

$\mathcal{H}(S_j)$: 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)

$$z_0 = \exp\left[A \overbrace{(S_1 S_2 + S_2 S_3 + S_3 S_4 + S_1 S_4)}^{\text{nearest neighbour terms}} + B \overbrace{(S_1 S_3 + S_2 S_4)}^{\text{next nearest neighbour terms}} + C S_1 S_2 S_3 S_4 + D\right]$$

- 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

factor ½ to account for relative numbers of terms

$$z_0 \to \overline{z_0} = \exp\left[\left(A + \frac{B}{2}\right)(S_1 S_2 + S_2 S_3 + S_3 S_4 + S_1 S_4) + D\right]$$

- in the full partition function a term, such as $\exp\left[\left(A + \frac{B}{2}\right) S_1 S_2\right]$ 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:

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

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

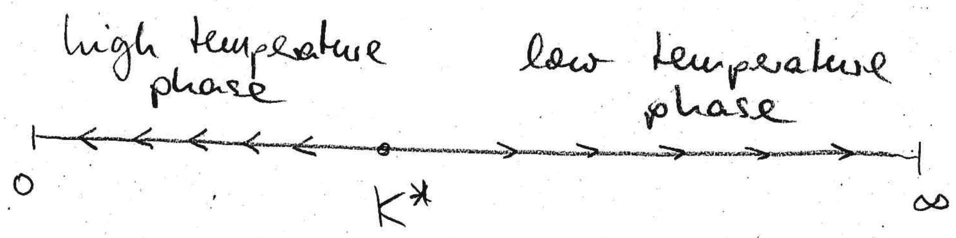
- this map has a fixed point at $K^* = 0.507$, which marks the critical coupling strength

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

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

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 $b = \sqrt{2}$

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

- 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 ($\frac{1}{D_{\bar{K}}} \approx 1.07$)