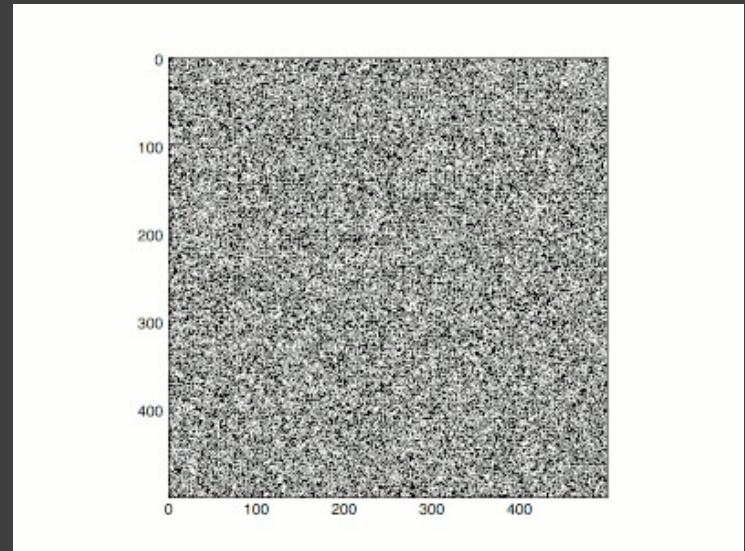




Ciências
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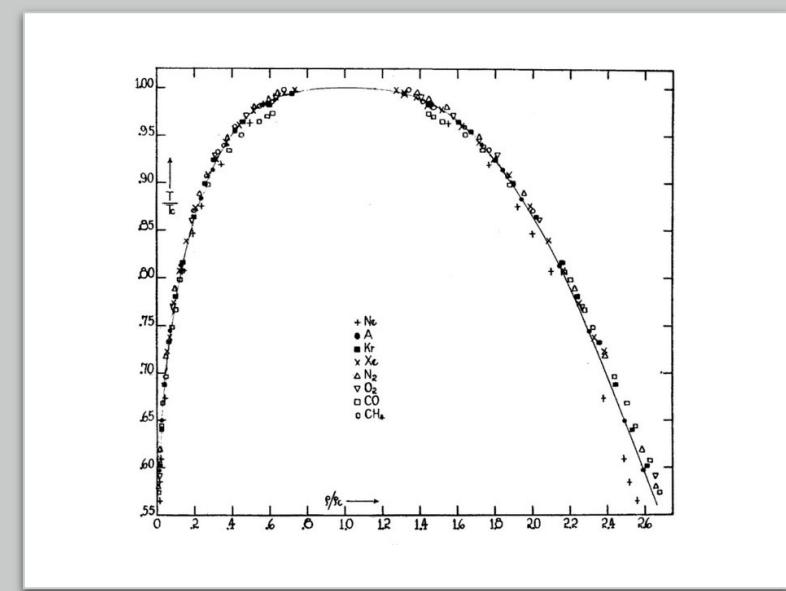
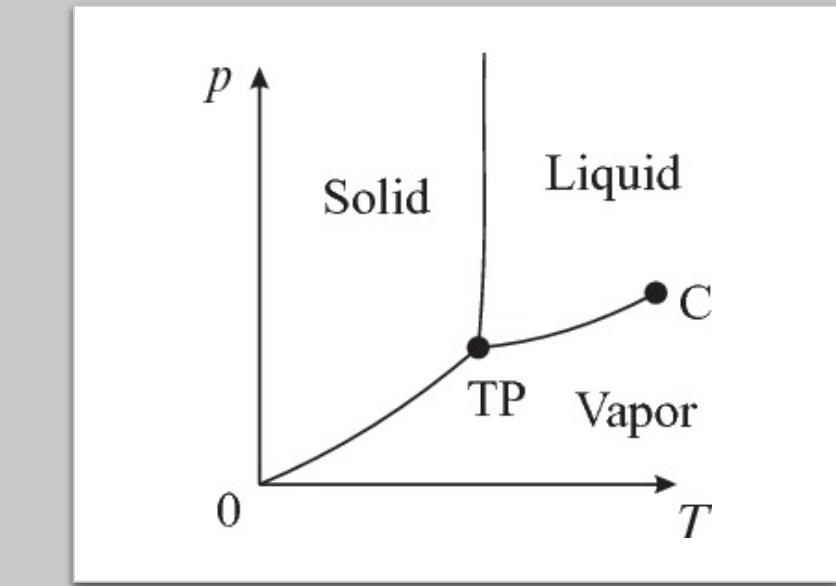
Ising Model

Criticality

Criticality refers to the behaviour of extended systems at a phase transition where no characteristic scale exists. Thermodynamically, a phase transition occurs when there is a singularity in the free energy. The liquid-gas, conductor-superconductor, fluid-superfluid, or paramagnetic-ferromagnetic phase transitions are common examples.

The Ising model of a ferromagnet is one of the simplest models displaying the paramagnetic-ferromagnetic phase transition, that is, the spontaneous emergence of magnetisation in zero external field as the temperature is lowered below a certain critical temperature.

At the critical point of critical temperature and zero-external field there is no characteristic scale. As in the case of percolation, the scale invariance is intimately related to fixed points of a rescaling transformation.



Ferro to paramagnetic phase transition

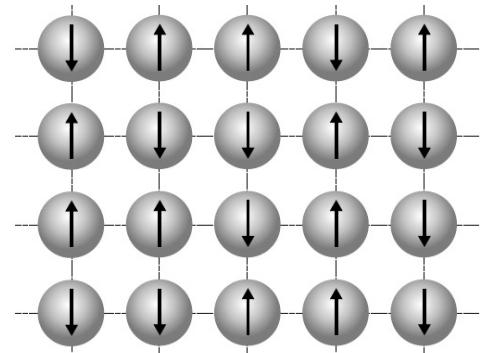
The paradigm of critical phase transitions is the transition from the paramagnetic state of iron to the ferromagnetic state, at the Curie temperature, $T_c = 1043$ K.

The spin of each iron atom has a particular orientation, corresponding to the direction of its local magnetic field.

Above T_c , the spins point in different directions and their magnetic fields are canceled. This disordered configuration is caused by the random thermal movement of the spins. The higher the temperature, the more difficult it is for any orderly arrangement of spins to be maintained.

However, when the temperature drops, the spins align spontaneously. Instead of canceling each other out, the individual magnetic fields are added, producing a macroscopic magnetic field.

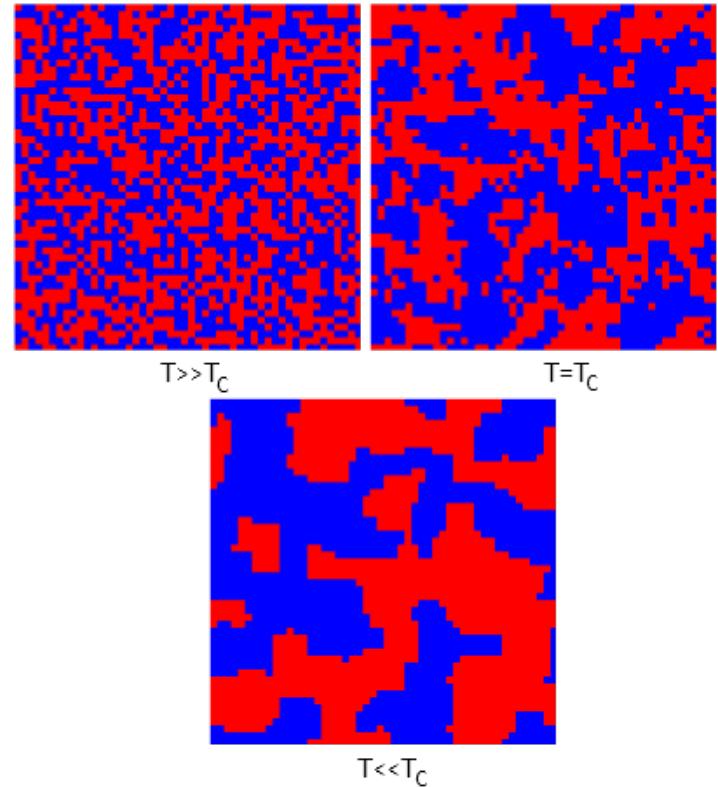
At T_c critical fluctuations lead to scaling and universality, i.e., the same power laws describe different ferromagnets.



Ising Model

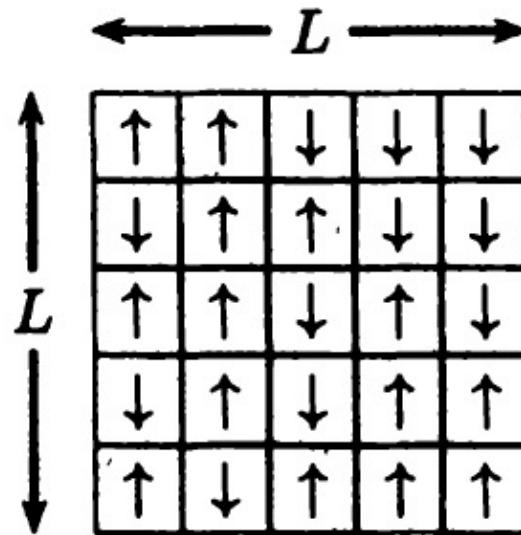
The Ising model has had an enormous impact on modern physics in general and statistical physics in particular, but also on other areas of science, including biology and neuroscience [Hopfield, 1982; Amit, 1989; Majewski et al., 2001], economics [Sornette, 2003] and sociology [Weidlich, 2001) among others. The importance of the Ising model cannot be overstated.

At present, hundreds of papers in these research areas are published each year on models inspired by the Ising model.



A microstate of the 2d Ising model on a lattice

Consider a 2d square lattice composed of $N = L \times L$ sites. Every site i is occupied by a spin, s_i . For a magnetic material, we may think of the spins as the magnetic dipoles positioned on the crystal structure lattice. In uniaxial magnetic materials, the magnetic dipole interactions constrain the spins to point parallel or anti-parallel along a given direction. Therefore, for simplicity, we assume that the spins can only be in one of two states, either spin-up, $s_i = +1$, or spin-down, $s_i = -1$.



Spin-spin and external interactions

i	j	s_i	s_j	interaction energy
↑	↑	+1	+1	$-J_{ij}$
↓	↓	-1	-1	$-J_{ij}$
↑	↓	+1	-1	$+J_{ij}$
↓	↑	-1	+1	$+J_{ij}$

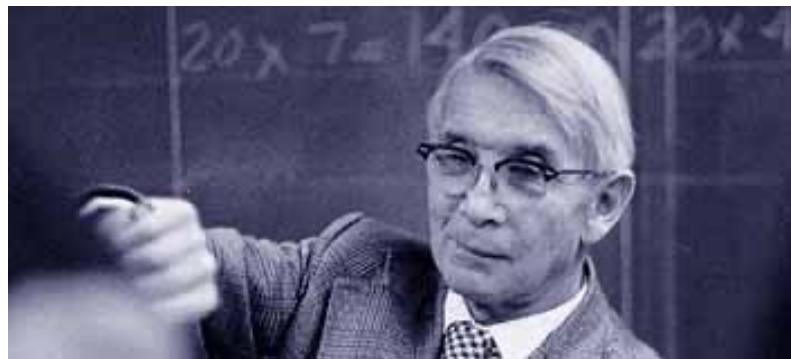
The spins at positions i and j interact with one another. For a pair of parallel spins we assign an interaction energy of $-J_{ij}$, while for a pair of anti-parallel spins we assign an interaction energy of $+J_{ij}$.

$$E_{\text{int}} = - \sum_{ij} J_{ij} s_i s_j,$$

In addition to the internal spin-spin interaction, we can impose a uniform external field, H, which acts upon every spin. A spin aligned parallel with the external field has energy $-HS_i$ associated with the spin-external field interaction, while a spin aligned anti-parallel with the external field has energy $+HS_i$. The external energy for each spin is thus $-HS_i$.

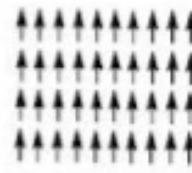
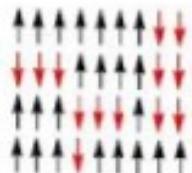
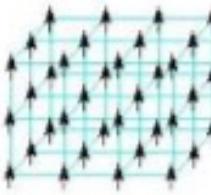
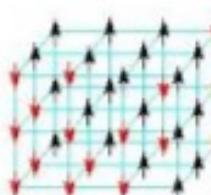
$$E_{\text{ext}} = -H \sum_{i=1}^N s_i,$$

Nearest-neighbour (single-coupling) Ising model



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

Ising Model

	Low T	High T	Solved
1-D			Ising – 1925
2-D			Onsager – 1944
3-D			Proven computationally intractable - 2000

As T increases, S increases but net magnetization decreases

Review of Statistical Mechanics

Statistical mechanics attempts to derive the thermodynamic laws of macroscopic quantities from a microscopic description of a system.

One can only measure the temporal average of a macroscopic observable. Microscopically, the temporal average of an observable is identified as a suitably weighted ensemble average, $\langle A \rangle$, over all possible microstates. Therefore, if $p_{\{s_i\}}$ is the probability of the system being in a particular microstate $\{s_i\}$ with observable $A_{\{s_i\}}$, its ensemble average is over 2^N configurations or microstates.

$$\langle A \rangle = \sum_{\{s_i\}} p_{\{s_i\}} A_{\{s_i\}},$$

$$\sum_{\{s_i\}} = \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} .$$

Boltzmann distribution



In the canonical ensemble the temperature and volume of the system are kept fixed. The probability $p_{\{s_i\}}$ to find the system in a microstate $\{s_i\}$ with energy $E_{\{s_i\}}$ is given by the Boltzmann distribution:

$$p_{\{s_i\}} = \frac{\exp(-\beta E_{\{s_i\}})}{\sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}})},$$

$$\langle A \rangle = \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) A_{\{s_i\}},$$

$$Z(T, H, N) = \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}),$$

The partition function Z is a suitably weighted average over all the possible microstates and provides the link between the microscopic and macroscopic descriptions of a system. The partition function depends on the temperature T , the external field H , and the number of spins N . Therefore, all ensemble averages of observables also depend on T , H , and N .

Magnetization

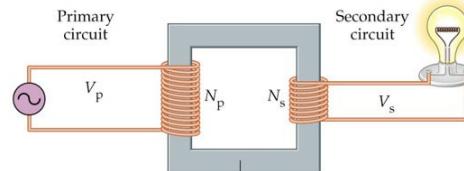
$$M_{\{s_i\}} = \sum_{i=1}^N s_i$$

$$\langle M \rangle = \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}}.$$



Energy

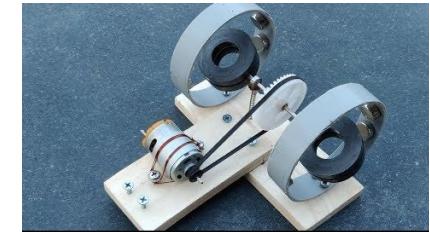
$$\langle E \rangle = \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) E_{\{s_i\}}.$$



Free energy

$$F(T, H) = -k_B T \ln Z.$$

$$F = \langle E \rangle - TS,$$



Ensemble average & free energy

Magnetization per spin

$$\begin{aligned}-N \left(\frac{\partial f}{\partial H} \right)_T &= k_B T \frac{\partial}{\partial H} \ln Z \\&= k_B T \frac{1}{Z} \frac{\partial}{\partial H} Z \\&= k_B T \frac{1}{Z} \frac{\partial}{\partial H} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\&= \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}}\end{aligned}$$

$$m(T, H) = - \left(\frac{\partial f}{\partial H} \right)_T ,$$

Response function: susceptibility

what are other
words for
susceptibility?

sensitivity, vulnerability,
sensitiveness, susceptibility,
liability, responsiveness,
openness, exposure, sensibility



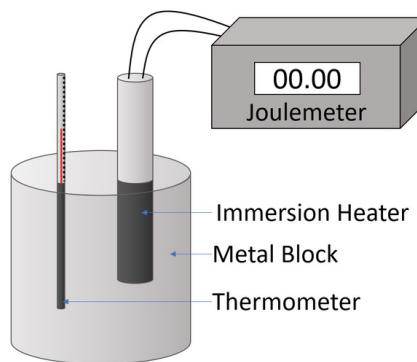
Thesaurus.plus

$$\begin{aligned}
 N\chi &= \left(\frac{\partial \langle M \rangle}{\partial H} \right)_T \\
 &= \frac{\partial}{\partial H} \left(\frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \right) \\
 &= \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \beta M_{\{s_i\}}^2 - \frac{1}{Z^2} \frac{\partial Z}{\partial H} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \\
 &= \beta \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}}^2 - \beta \left(\frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) M_{\{s_i\}} \right)^2 \\
 &= \beta \left(\langle M^2 \rangle - \langle M \rangle^2 \right). \tag{2.19}
 \end{aligned}$$

$$\chi(T, H) = \left(\frac{\partial m}{\partial H} \right)_T,$$

$$k_B T \chi = \frac{1}{N} \left(\langle M^2 \rangle - \langle M \rangle^2 \right).$$

Response function: specific heat



$$c(T, H) = \left(\frac{\partial \epsilon}{\partial T} \right)_H ,$$

$$k_B T^2 c = \frac{1}{N} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) .$$

Summary

Quantity	Relation	Response function
Partition function:	$Z = \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}})$	
Free energy per spin:	$f = -\frac{1}{N} k_B T \ln Z$	
Magnetisation per spin:	$m = -\left(\frac{\partial f}{\partial H}\right)_T$	$\chi = \left(\frac{\partial m}{\partial H}\right)_T = -\left(\frac{\partial^2 f}{\partial H^2}\right)_T$
Energy per spin:	$\varepsilon = -\frac{1}{N} \left(\frac{\partial \ln Z}{\partial \beta}\right)_H = f - T \left(\frac{\partial f}{\partial T}\right)_H$	$c = \left(\frac{\partial \varepsilon}{\partial T}\right)_H = -T \left(\frac{\partial^2 f}{\partial T^2}\right)_H$
Entropy per spin:	$S/N = -\left(\frac{\partial f}{\partial T}\right)_H = \frac{1}{T} (\varepsilon - f)$	

Thermodynamic limit

Specifically, in d dimensions, the total free energy F for a finite system of $N = L^d$ spins can be separated into a bulk contribution, F_{bulk} , and a boundary contribution, F_{boundary} , which are proportional to L^d and L^{d-1} respectively. When considering the free energy per spin, boundary effects decrease with increasing system size and disappear altogether in the thermodynamic limit. Therefore, in the thermodynamic limit, the free energy of the system per spin reduces to the bulk free energy per spin,

$$\lim_{N \rightarrow \infty} \frac{F}{N} = \lim_{N \rightarrow \infty} \frac{F_{\text{bulk}} + F_{\text{boundary}}}{N} = \lim_{N \rightarrow \infty} \frac{F_{\text{bulk}}}{N}.$$

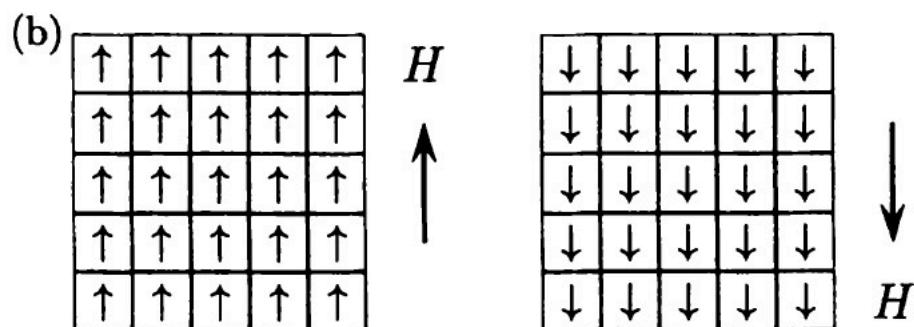
In the thermodynamic limit, there is an infinite number of terms in the partition function. In this case, the free energy is no longer guaranteed to be analytic, and there is at least a possibility that it is not.

Non-interacting (independent) spins

$$E_{\{s_i\}} = -H \sum_{i=1}^N s_i.$$

(a)

↑	↑	↓	↓	↓
↓	↑	↑	↓	↓
↑	↑	↓	↑	↓
↓	↑	↓	↑	↑
↑	↓	↑	↑	↑

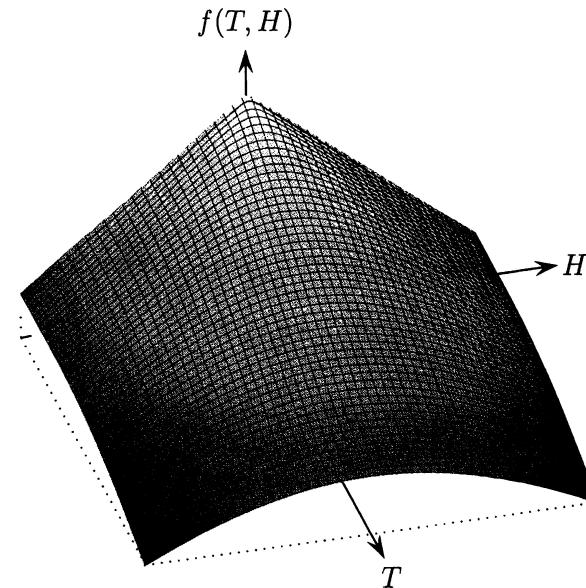


$$\begin{aligned}
Z(T, H) &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\
&= \sum_{\{s_i\}} \exp\left(\beta H \sum_{i=1}^N s_i\right) \\
&= \sum_{\{s_i\}} \exp(\beta H s_1) \exp(\beta H s_2) \cdots \exp(\beta H s_N) \\
&= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} \exp(\beta H s_1) \exp(\beta H s_2) \cdots \exp(\beta H s_N) \\
&= \sum_{s_1=\pm 1} \exp(\beta H s_1) \sum_{s_2=\pm 1} \exp(\beta H s_2) \cdots \sum_{s_N=\pm 1} \exp(\beta H s_N) \\
&= (\exp(\beta H) + \exp(-\beta H))^N \\
&= (2 \cosh \beta H)^N.
\end{aligned} \tag{2.25}$$

$$\begin{aligned}
F(T, H) &= -k_B T \ln (2 \cosh \beta H)^N \\
&= -N k_B T \ln (2 \cosh \beta H).
\end{aligned}$$

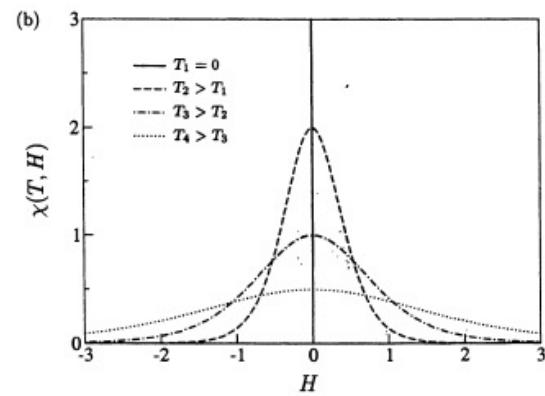
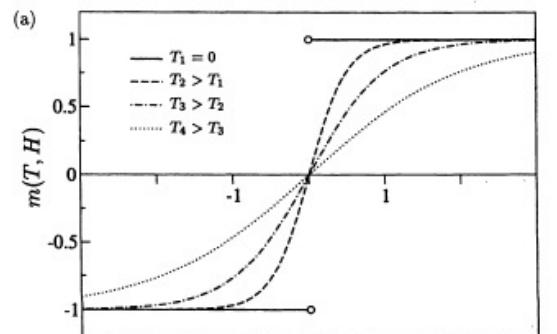
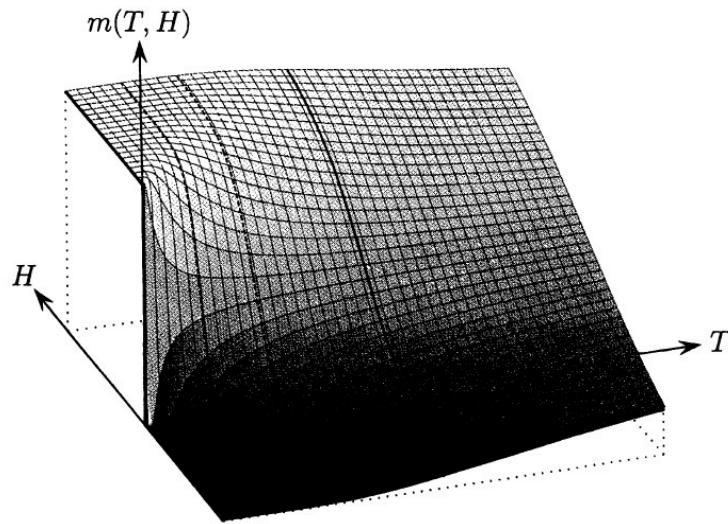
$$f(T, H) = -k_B T \ln (2 \cosh \beta H).$$

Free energy density



Magnetization & susceptibility

$$m(T, H) = - \left(\frac{\partial f}{\partial H} \right)_T = k_B T \frac{2 \sinh \beta H}{2 \cosh \beta H} \quad \beta = \tanh \beta H.$$



Fluctuations of the magnetization

Susceptibility

$$\chi(T, H) = \left(\frac{\partial m}{\partial H} \right)_T = \beta \operatorname{sech}^2 \beta H$$

$$\chi(T, 0) = \frac{1}{k_B T}.$$

Fluctuations in the magnetization

$$k_B T \chi = \operatorname{sech}^2 \beta H = \frac{1}{N} \left(\langle M^2 \rangle - \langle M \rangle^2 \right),$$

$$\frac{\sqrt{\langle M^2 \rangle - \langle M \rangle^2}}{\langle M \rangle} = \frac{1}{\sqrt{N}} \operatorname{csch} \beta H \propto \frac{1}{\sqrt{N}} \quad \text{for } H \neq 0.$$

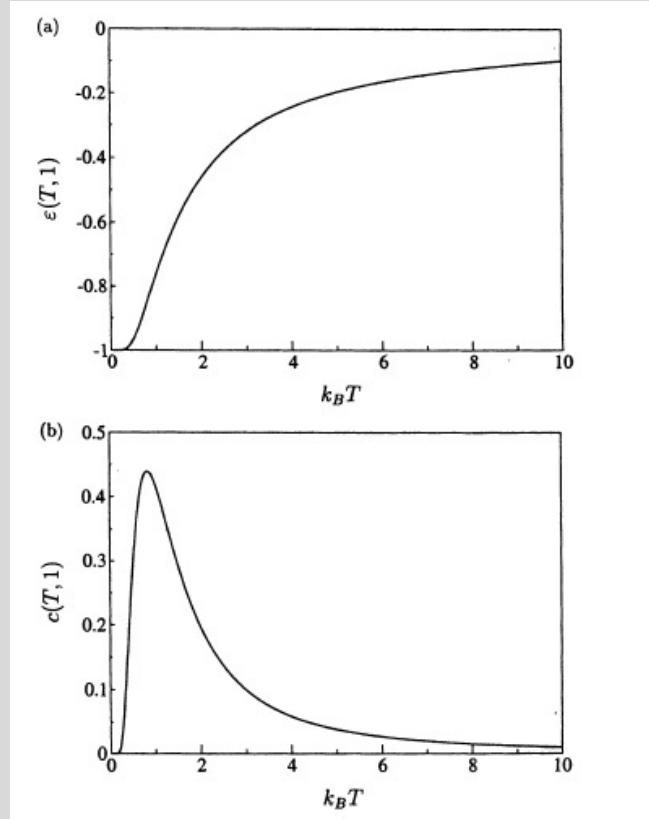
Average energy & specific heat

Average energy

$$\varepsilon(T, H) = -\frac{1}{N} \left(\frac{\partial \ln Z}{\partial \beta} \right)_H = -\frac{2 \sinh \beta H}{2 \cosh \beta H} H = -H \tanh \beta H;$$

Specific heat

$$c(T, H) = \left(\frac{\partial \varepsilon}{\partial T} \right)_H = -H \operatorname{sech}^2(\beta H) \frac{-H}{k_B T^2} = \frac{H^2}{k_B T^2} \operatorname{sech}^2 \beta H;$$



Fluctuations of the energy

$$k_B T^2 c = H^2 \operatorname{sech}^2 \beta H = \frac{1}{N} \left(\langle E^2 \rangle - \langle E \rangle^2 \right),$$

$$\frac{\sqrt{\langle E^2 \rangle - \langle E \rangle^2}}{\langle E \rangle} = -\frac{\operatorname{sign}(H)}{\sqrt{N}} \operatorname{csch} \beta H \propto \frac{1}{\sqrt{N}} \quad \text{for } H \neq 0.$$

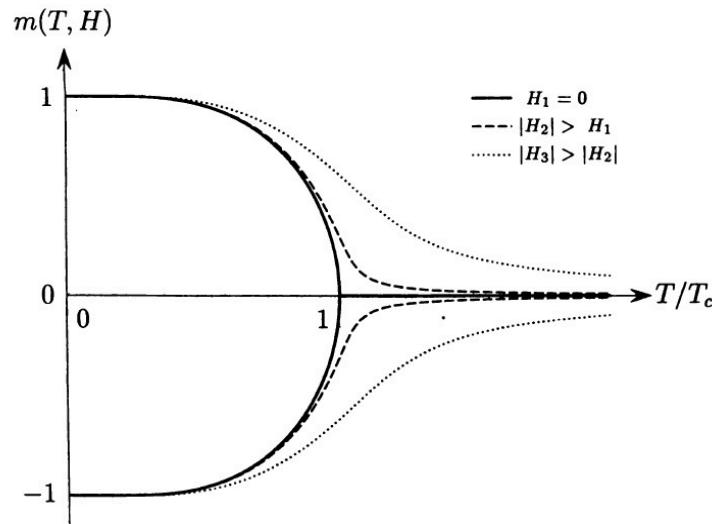
Interacting spins



Expectations

$$m_0(T) = \lim_{H \rightarrow 0^\pm} m(T, H) \propto \begin{cases} 0 & \text{for } T \geq T_c \\ \pm(T_c - T)^\beta & \text{for } T \rightarrow T_c^-, \end{cases}$$

$$m(T_c, H) \propto \text{sign}(H)|H|^{1/\delta} \quad \text{for } |H| \rightarrow 0, T = T_c,$$



Ising model

Magnetization
exponents β & δ

Ising model

Response functions

$$\chi(T, 0) \propto |T - T_c|^{-\gamma} \quad \text{for } T \rightarrow T_c.$$

$$c(T, 0) \propto |T - T_c|^{-\alpha} \quad \text{for } T \rightarrow T_c.$$

Correlation length

$$\xi(T, 0) \propto |T - T_c|^{-\nu} \quad \text{for } T \rightarrow T_c.$$

Response
function
exponents γ & α

&

Correlation
length exponent
 ν

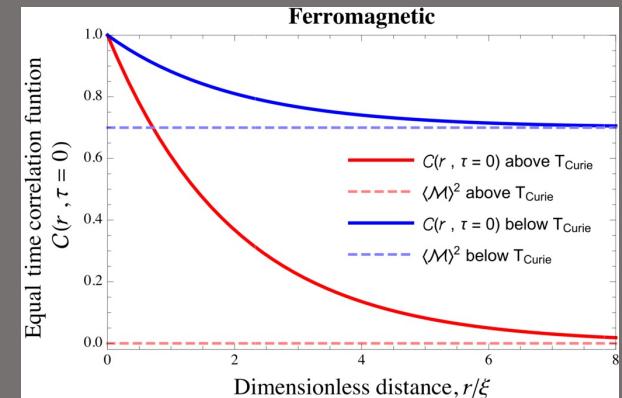
The spin-spin correlation function

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle \\ &= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle, \end{aligned}$$

$$\begin{aligned} Nk_B T \chi &= \langle M^2 \rangle - \langle M \rangle^2 \\ &= \left\langle \sum_{k=1}^N s_k \sum_{j=1}^N s_j \right\rangle - \left\langle \sum_{k=1}^N s_k \right\rangle \left\langle \sum_{j=1}^N s_j \right\rangle \\ &= \sum_{k=1}^N \sum_{j=1}^N (\langle s_k s_j \rangle - \langle s_k \rangle \langle s_j \rangle) \\ &= \sum_{k=1}^N \sum_{j=1}^N g(\mathbf{r}_k, \mathbf{r}_j) \\ &= N \sum_{j=1}^N g(\mathbf{r}_i, \mathbf{r}_j), \end{aligned}$$

Ising model

Correlation function



Ising model

Sum rule

$$\int_V g(\mathbf{r}_i, \mathbf{r}_j) d\mathbf{r}_j = k_B T \chi.$$

At T_c the correlation function decays as a power law

$$g(\mathbf{r}_i, \mathbf{r}_j) \propto r^{-(d-2+\eta)} \quad \text{for } (T, H) = (T_c, 0),$$

Correlation
function
exponent η

Critical Exponents of the Ising Model

dimensions	2	3	≥ 4 **
ν	1	0.6301	$1/2$
γ	$7/4$	1.2373	1
α	logarithmic	0.110	
β^*	$1/8$	0.3265	$1/2$
δ	15	4.789	3
η	$1/4$	0.0365	

* the beta exponent here is not the inverse temperature

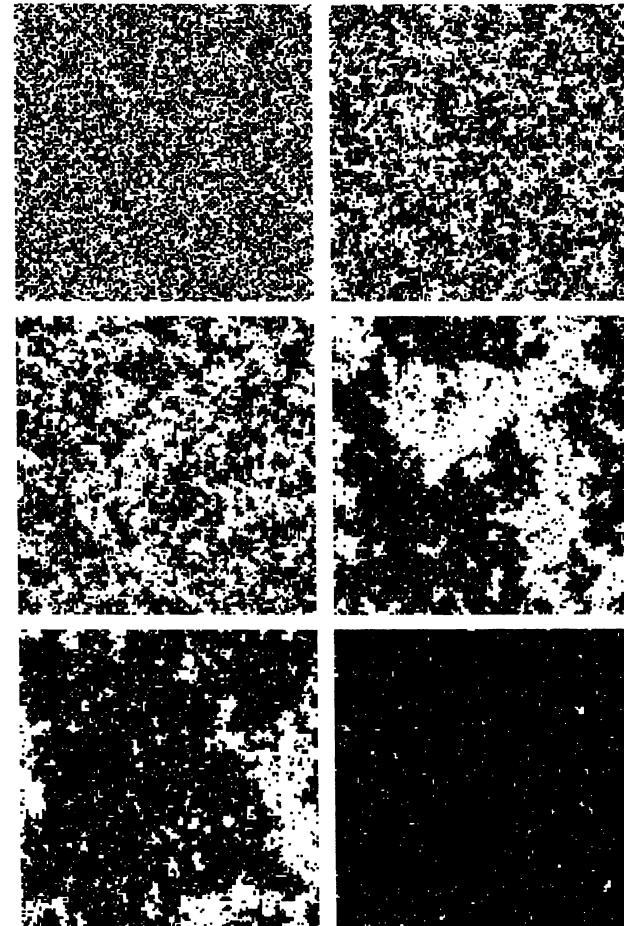
** exact results from mean field-theory

Configurations

Six microstates of the 2d Ising model on a square lattice of size $L = 150$ for six different temperatures in zero external field, $H = 0$.

At relatively high temperatures $T \gg T_c$, the spins are randomly orientated with no correlations. As the temperature is lowered, the spin-spin interactions are less suppressed so that larger and larger clusters of correlated spins form.

At $T = T_c$, a macroscopic cluster of correlated spins appears for the first time. This cluster is fractal and contains clusters of all sizes of opposite spins, which themselves contain clusters of all sizes of opposite spins, and so on, like droplets within droplets ...



Symmetry breaking

The probabilities of finding the system in the microstates $\{s_i\}$ and $\{-s_i\}$ are

$$p_{\{s_i\}} = \frac{\exp(-\beta E_{\{s_i\}})}{Z},$$
$$p_{\{-s_i\}} = \frac{\exp(-\beta E_{\{-s_i\}})}{Z},$$

$$\frac{p_{\{s_i\}}}{p_{\{-s_i\}}} = \exp [-\beta (E_{\{s_i\}} - E_{\{-s_i\}})].$$

In zero external field, the energy of a spin configuration is invariant if all the spins are reversed:

$$E_{\{s_i\}} - E_{\{-s_i\}} = 0, \quad \text{for } H = 0.$$

The magnetisation changes sign if all the spins are reversed:

$$M_{\{s_i\}} = -M_{\{-s_i\}}.$$

$$\langle M \rangle = \sum_{\{s_i\}} p_{\{s_i\}} M_{\{s_i\}} = 0,$$

Have we just proved that the average total magnetisation in the Ising model is always zero in zero external field, thereby destroying the possibility of a phase transition? To answer this question negatively, we first consider the effect of introducing a small non-zero external field. Explicitly, the energy difference

$$E_{\{s_i\}} - E_{\{-s_i\}} = -2H \sum_{i=1}^N s_i = -2HM_{\{s_i\}},$$

$$\frac{p_{\{s_i\}}}{p_{\{-s_i\}}} = \exp(2\beta HM_{\{s_i\}}).$$

Without loss of generality, assume that $M\{s_i\} > 0$. Taking the external field to zero before taking the thermodynamic limit, we find that

$$\lim_{N \rightarrow \infty} \lim_{H \rightarrow 0^\pm} \frac{p_{\{s_i\}}}{p_{\{-s_i\}}} = 1.$$

On the other hand, taking the thermodynamic limit before taking the external field to zero, we find that

$$\lim_{H \rightarrow 0^\pm} \lim_{N \rightarrow \infty} \frac{p_{\{s_i\}}}{p_{\{-s_i\}}} = \begin{cases} \infty & \text{for } H \rightarrow 0^+ \\ 0 & \text{for } H \rightarrow 0^- \end{cases}$$

The existence of a non-zero external field, however small, therefore breaks the symmetry among the spin configurations.

The thermodynamic limit and the limit of vanishing external field are not interchangeable, that is,

$$\lim_{N \rightarrow \infty} \lim_{H \rightarrow 0^\pm} \langle M \rangle = 0,$$
$$\lim_{H \rightarrow 0^\pm} \lim_{N \rightarrow \infty} \langle M \rangle \neq 0.$$

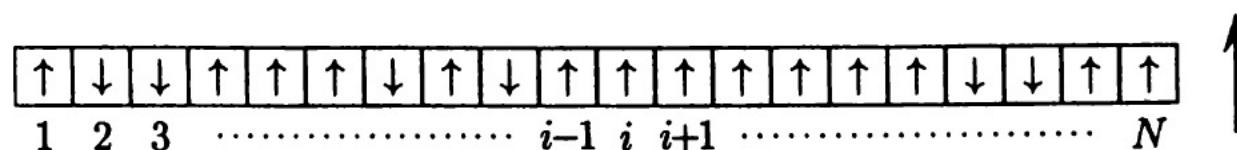
In the thermodynamic limit, the ergodicity of the system is said to be 'spontaneously broken' for $T < T_c$, and it is this that gives rise to a nonzero magnetisation.

1d Ising model

In $d = 1$ the total energy of the Ising model for N spins in a uniform external field H is

$$\begin{aligned} E_{\{s_i\}} &= -J \sum_{\langle ij \rangle} s_i s_j - H \sum_{i=1}^N s_i \\ &= -J \sum_{i=1}^N s_i s_{i+1} - H \sum_{i=1}^N s_i, \end{aligned}$$

Periodic boundary conditions are applied, $s_1 = s_{N+1}$



Partition function

$$\begin{aligned} Z &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\ &= \sum_{\{s_i\}} \exp \left(\beta J \sum_{i=1}^N s_i s_{i+1} + \beta H \sum_{i=1}^N s_i \right) \\ &= \sum_{\{s_i\}} \exp \left(\beta J \sum_{i=1}^N s_i s_{i+1} + \beta \frac{H}{2} \sum_{i=1}^N (s_i + s_{i+1}) \right) \quad (2.59) \\ &= \sum_{\{s_i\}} \exp \left(\beta J s_1 s_2 + \beta \frac{H}{2} (s_1 + s_2) \right) \cdots \exp \left(\beta J s_N s_1 + \beta \frac{H}{2} (s_N + s_1) \right). \end{aligned}$$

Transfer matrix method

There are four possible configurations of the two spins s_i and s_{i+1} , and it is convenient to arrange these in a real and symmetric 2×2 transfer matrix, T , with entries:

$$T_{s_i s_{i+1}} = \exp \left(\beta J s_i s_{i+1} + \beta \frac{H}{2} (s_i + s_{i+1}) \right),$$

$$\mathbf{T} = \begin{pmatrix} T_{+1+1} & T_{+1-1} \\ T_{-1+1} & T_{-1-1} \end{pmatrix} = \begin{pmatrix} \exp(\beta J + \beta H) & \exp(-\beta J) \\ \exp(-\beta J) & \exp(\beta J - \beta H) \end{pmatrix}.$$

$$\begin{aligned} Z &= \sum_{\{s_i\}} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_{N-1} s_N} T_{s_N s_1} \\ &= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_N=\pm 1} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_{N-1} s_N} T_{s_N s_1} \tag{2.62} \\ &= \sum_{s_1=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \left(\sum_{s_2=\pm 1} T_{s_1 s_2} T_{s_2 s_3} \right) \cdots \left(\sum_{s_N=\pm 1} T_{s_{N-1} s_N} T_{s_N s_1} \right). \end{aligned}$$

$$A_{ij}^2 = \sum_{k=1}^n A_{ik} A_{kj}.$$

We can therefore rewrite the sum over paired terms as entries from their product matrix T^2 ,

$$\begin{aligned} Z &= \sum_{s_1=\pm 1} \sum_{s_3=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} T_{s_1 s_3}^2 T_{s_3 s_5}^2 \cdots T_{s_{N-3} s_{N-1}}^2 T_{s_{N-1} s_1}^2 \\ &= \sum_{s_1=\pm 1} \sum_{s_5=\pm 1} \cdots \sum_{s_{N-3}=\pm 1} T_{s_1 s_5}^4 T_{s_5 s_9}^4 \cdots T_{s_{N-7} s_{N-3}}^4 T_{s_{N-3} s_1}^4 \\ &= \sum_{s_1=\pm 1} T_{s_1 s_1}^N \\ &= \text{Tr}(\mathbf{T}^N), \end{aligned}$$

The final expression is the trace of \mathbf{T}^N , that is, the sum over the diagonal elements of the matrix \mathbf{T}^N . For the trace we only need the diagonal elements rather than the whole matrix. We use a result from linear algebra which states that for the real and symmetric 2×2 matrix T there exists a 2×2 unitary matrix U , such that

$$\mathbf{U}^{-1} \mathbf{T} \mathbf{U} = \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix}, \quad \det(\mathbf{T} - \lambda \mathbf{I}) = 0,$$

$$\lambda_{\pm} = \exp(\beta J) \left(\cosh \beta H \pm \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} \right)$$

Using the identity $UU^{-1} = I$ and the commutative property of the trace operation, $\text{Tr}(AB) = \text{Tr}(BA)$, the partition function is therefore

$$\begin{aligned}
Z &= \text{Tr}(\mathbf{T}^N) \\
&= \text{Tr}(\mathbf{T}\mathbf{U}\mathbf{U}^{-1}\mathbf{T}\mathbf{U}\mathbf{U}^{-1}\cdots\mathbf{T}\mathbf{U}\mathbf{U}^{-1}) \\
&= \text{Tr}(\underbrace{(\mathbf{U}^{-1}\mathbf{T}\mathbf{U})(\mathbf{U}^{-1}\mathbf{T}\mathbf{U})\cdots(\mathbf{U}^{-1}\mathbf{T}\mathbf{U})}_{N\text{factors}}) \\
&= \text{Tr}\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix} \\
&= \lambda_+^N + \lambda_-^N.
\end{aligned}$$

For zero external field $H = 0$, the partition function is

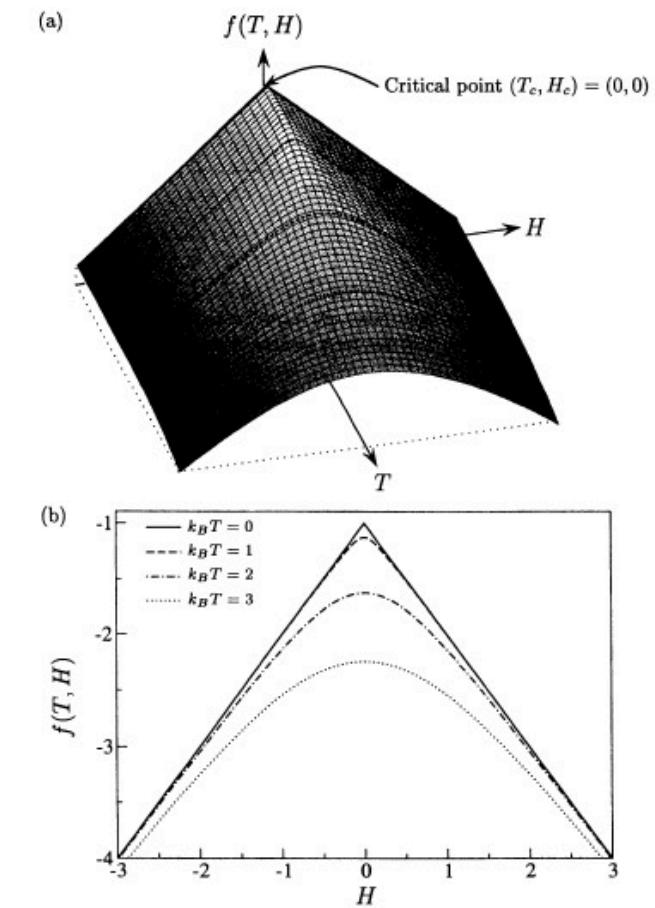
$$Z(T, 0) = (2 \cosh \beta J)^N (1 + \tanh^N \beta J) \rightarrow (2 \cosh \beta J)^N \text{ for } N \rightarrow \infty$$

The total free energy is

$$\begin{aligned}
F &= -k_B T \ln Z \\
&= -k_B T \ln \left(\lambda_+^N \left[1 + \left(\frac{\lambda_-}{\lambda_+} \right)^N \right] \right) \\
&= -k_B T \ln \lambda_+^N \text{ for } N \rightarrow \infty \\
&= -N k_B T \left[\beta J + \ln \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} \right) \right].
\end{aligned}$$

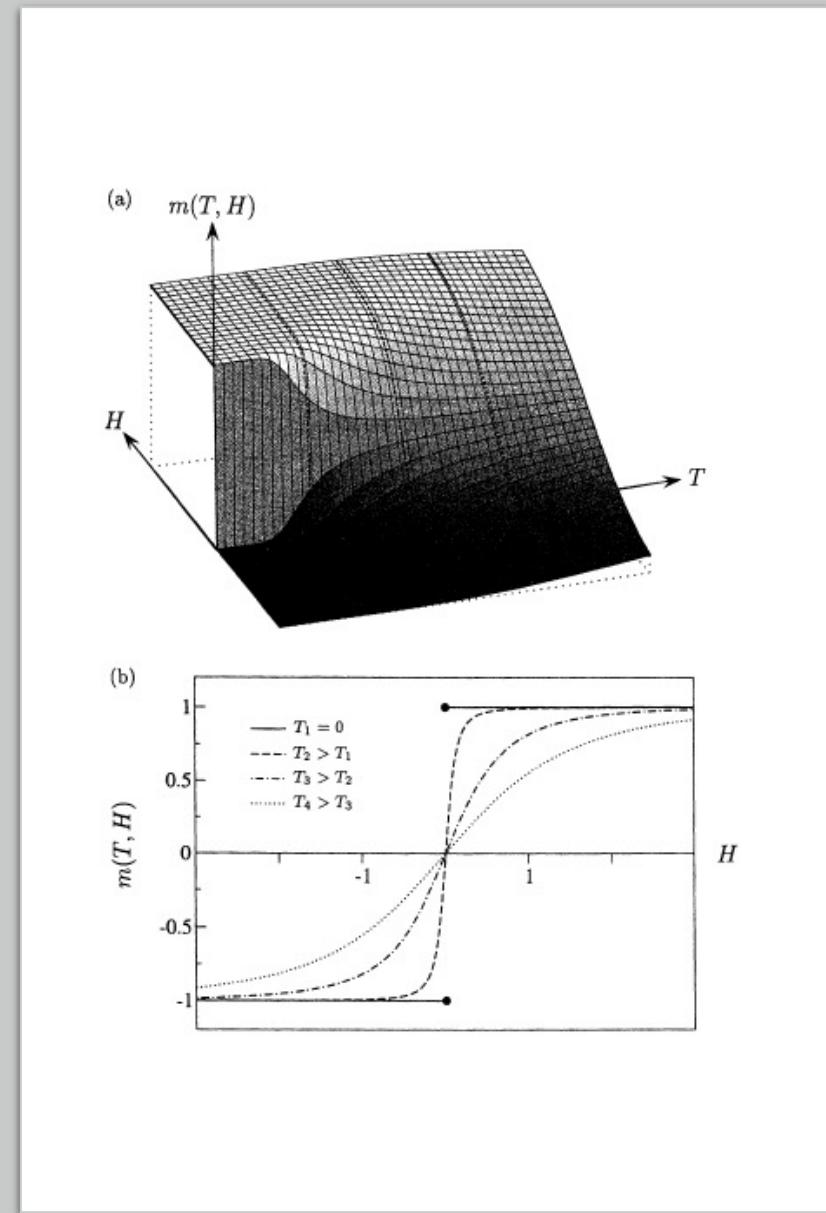
Free energy density

$$f(T, 0) = -k_B T \ln(2 \cosh \beta J) \rightarrow \begin{cases} -k_B T \ln 2 & \text{for } T \rightarrow \infty \\ -J & \text{for } T \rightarrow 0. \end{cases}$$



Magnetization per spin

$$\begin{aligned}
 m(T, H) &= - \left(\frac{\partial f}{\partial H} \right)_T \\
 &= k_B T \frac{\beta \sinh \beta H + \frac{2\beta \sinh \beta H \cosh \beta H}{2\sqrt{\sinh^2 \beta H + \exp(-4\beta J)}}}{\cosh \beta H + \sqrt{\sinh^2 \beta H + \exp(-4\beta J)}} \\
 &= \frac{\sinh \beta H}{\sqrt{\sinh^2 \beta H + \exp(-4\beta J)}}.
 \end{aligned}$$



Susceptibility

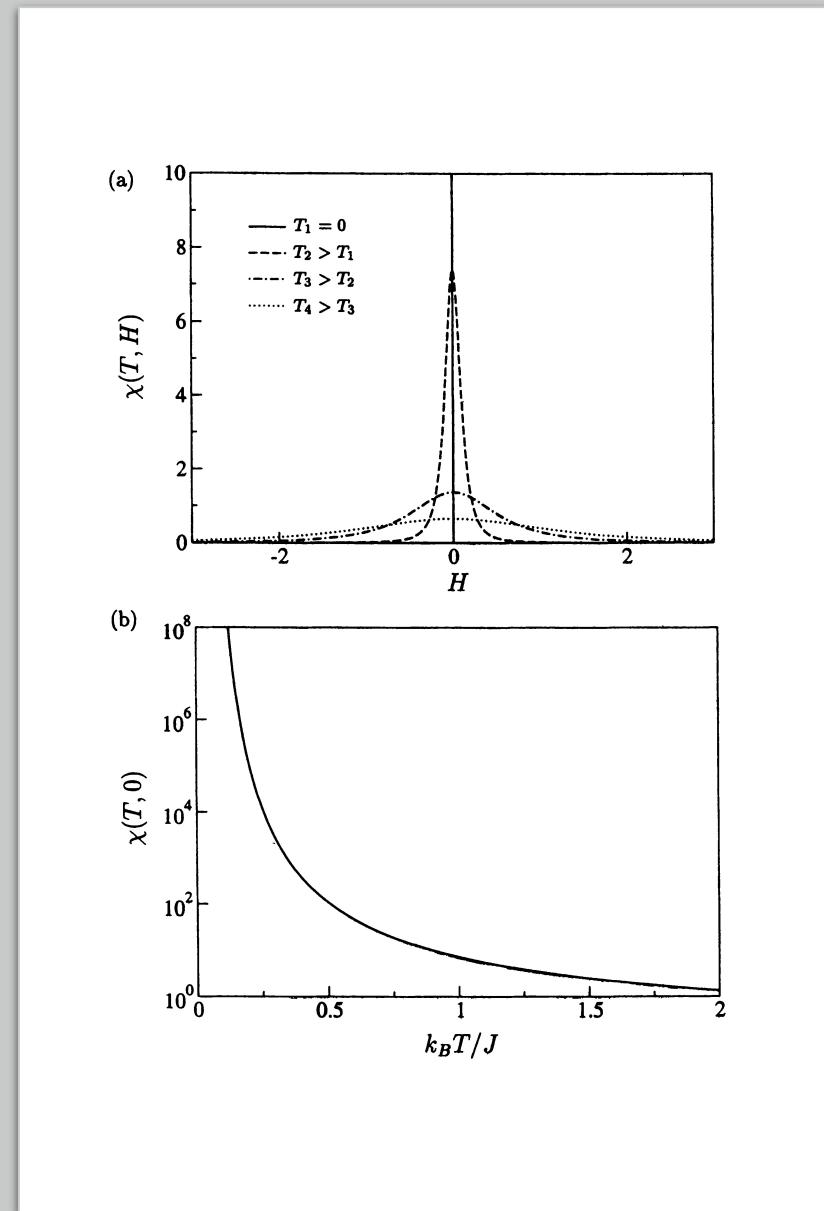
$$\begin{aligned}
 \chi(T, H) &= \left(\frac{\partial m}{\partial H} \right)_T \\
 &= \beta \frac{\cosh \beta H \sqrt{\sinh^2 \beta H + \exp(-4\beta J)} - \sinh \beta H \frac{\sinh \beta H \cosh \beta H}{\sqrt{\sinh^2 \beta H + \exp(-4\beta J)}}}{\sinh^2 \beta H + \exp(-4\beta J)} \\
 &= \beta \frac{\cosh \beta H \exp(-4\beta J)}{[\sinh^2 \beta H + \exp(-4\beta J)]^{3/2}}. \tag{2.75}
 \end{aligned}$$

In zero field,

$$\chi(T, 0) = \beta \exp(2\beta J) \rightarrow \begin{cases} \beta & \text{for } T \rightarrow \infty \\ \beta \exp(2\beta J) & \text{for } T \rightarrow 0, \end{cases}$$

$$k_B T \chi(T, 0) = \exp(2\beta J).$$

The fluctuations in m diverge at $T = 0$ by contrast to the ideal paramagnet.

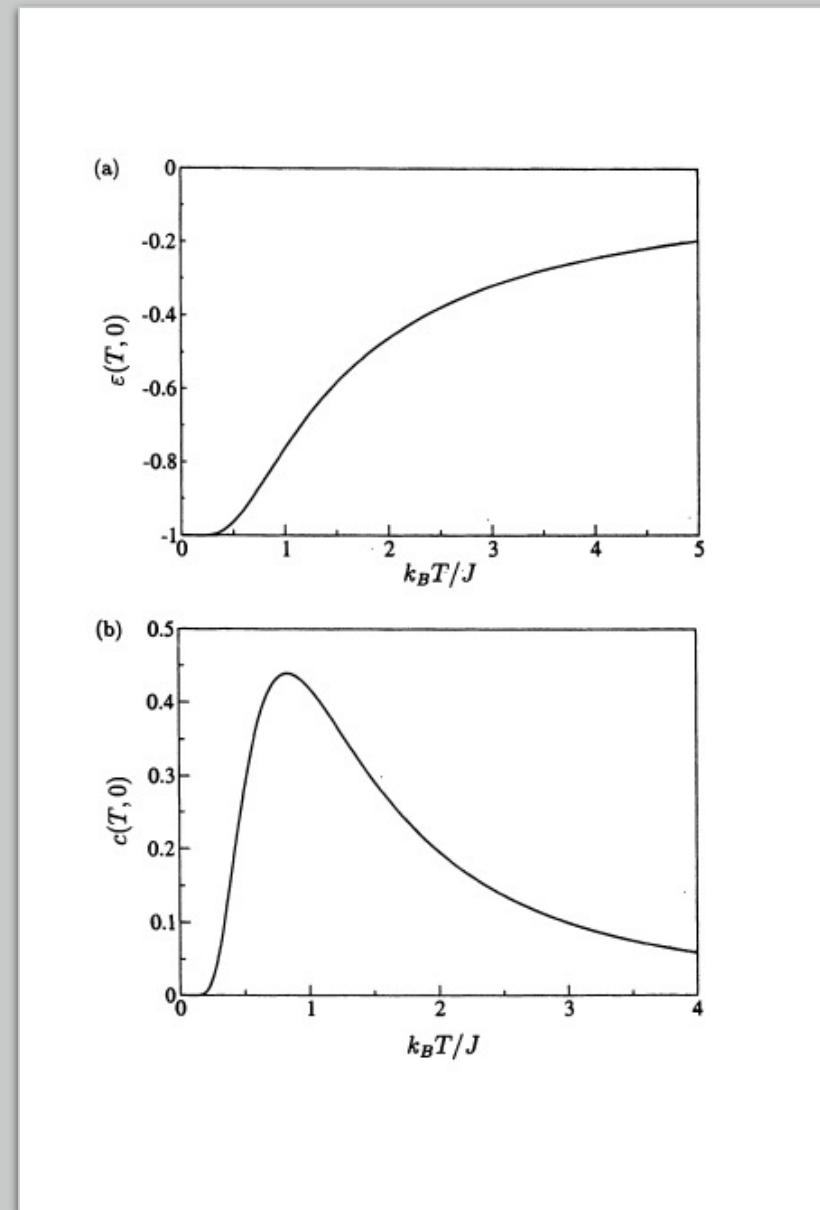


Energy & specific heat (zero field)

$$\begin{aligned}\epsilon(T, 0) &= -\frac{1}{N} \frac{\partial \ln Z(T, 0)}{\partial \beta} \\ &= -J \tanh \beta J \\ &\rightarrow \begin{cases} 0 & \text{for } T \rightarrow \infty \\ -J & \text{for } T \rightarrow 0; \end{cases}\end{aligned}$$

$$\begin{aligned}c(T, 0) &= \frac{\partial \epsilon(T, 0)}{\partial T} \\ &= \frac{\partial \epsilon}{\partial \beta} \frac{\partial \beta}{\partial T} \\ &= \frac{J^2}{k_B T^2} \operatorname{sech}^2 \beta J.\end{aligned}$$

$$k_B T^2 c(T, 0) = J^2 \operatorname{sech}^2 \beta J,$$



Correlation function

The spin-spin correlation function

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle \\ &= \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \end{aligned}$$

The Ising model is translationally and rotationally invariant:

$$g(\mathbf{r}_i, \mathbf{r}_j) = \langle s_i s_{i+r} \rangle - m^2.$$

$$g(\mathbf{r}_i, \mathbf{r}_j) = \langle s_i s_{i+r} \rangle - m_0^2(T) \quad \text{for } H = 0.$$

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \langle s_i s_{i+r} \rangle && \text{for } d = 1, T > 0, H = 0 \\ &= \frac{1}{Z} \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) s_i s_{i+r} && \text{for } d = 1, T > 0, H = 0. \end{aligned}$$

It is advantageous to assume, for the moment, that the nearest neighbour interactions depend on position

$$E_{\{s_i\}} = - \sum_{i=1}^N J_i s_i s_{i+1}. \quad Z = \prod_{i=1}^N 2 \cosh \beta J_i.$$

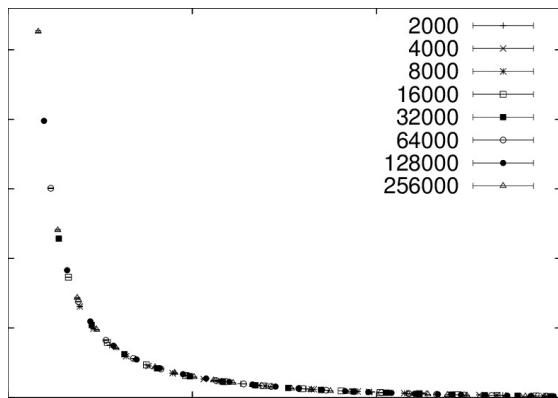
Correlation function

In the one-dimensional Ising model the spin-spin correlation function only depends on the distance between spins $r = |\mathbf{r}_i - \mathbf{r}_j|$, and decays exponentially with the correlation length in zero external field.

$$\begin{aligned} g(\mathbf{r}_i, \mathbf{r}_j) &= \frac{1}{Z} \sum_{\{s_i\}} \exp \left(\beta \sum_{i=1}^N J_i s_i s_{i+1} \right) s_i s_{i+r} \cdots \\ &= \frac{1}{Z} \sum_{\{s_i\}} \exp \left(\beta \sum_{i=1}^N J_i s_i s_{i+1} \right) s_i s_{i+1} s_{i+1} \cdots s_{i+r-1} s_{i+r-1} s_{i+r} \\ &= \frac{1}{Z} \sum_{\{s_i\}} \frac{1}{\beta^r} \frac{\partial^r}{\partial J_i \partial J_{i+1} \cdots \partial J_{i+r-1}} \exp \left(\beta \sum_{i=1}^N J_i s_i s_{i+1} \right) \\ &= \frac{1}{Z \beta^r} \frac{\partial^r}{\partial J_i \partial J_{i+1} \cdots \partial J_{i+r-1}} \sum_{\{s_i\}} \exp \left(\beta \sum_{i=1}^N J_i s_i s_{i+1} \right) \\ &= \frac{1}{Z \beta^r} \frac{\partial^r}{\partial J_i \partial J_{i+1} \cdots \partial J_{i+r-1}} \prod_{i=1}^N 2 \cosh \beta J_i \\ &= \frac{(2 \cosh \beta J)^{N-r} (2 \beta \sinh \beta J)^r}{(2 \cosh \beta J)^N \beta^r} \quad \text{after restoring } J_i = J \\ &= \tanh^r \beta J \\ &= \exp [r \ln (\tanh \beta J)]. \end{aligned} \tag{2.90}$$

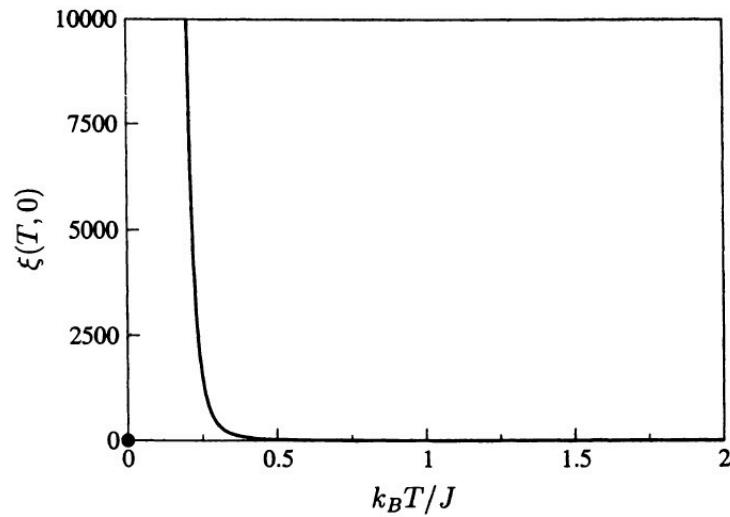
$$g(\mathbf{r}_i, \mathbf{r}_j) = \exp (-r/\xi) \quad \text{for } d = 1, T > 0, H = 0,$$

Correlation length



$$g(\mathbf{r}_i, \mathbf{r}_j) = \exp(-r/\xi) \quad \text{for } d = 1, T > 0, H = 0,$$

$$\xi(T, 0) = -\frac{1}{\ln(\tanh \beta J)} = \frac{1}{\ln(\lambda_+/\lambda_-)} \quad \text{for } d = 1,$$



Correlation length

At high temperatures, the spins are randomly orientated and thus uncorrelated.

The correlation length is zero and there are no fluctuations away from states with randomly orientated spins. As the temperature is decreased, spins align to form clusters of larger and larger size limited only by the correlation length.

For temperatures approaching zero, the correlation length diverges. Clusters of all sizes form and there are fluctuations of all scales away from states with randomly orientated spins.

However, at $T = 0$ all spins are aligned and the correlation length is zero.

$$\begin{aligned}\xi(T, 0) &= \frac{1}{\ln [\lambda_+ / \lambda_-]} \\ &= \frac{1}{\ln [(1 + \exp(-2\beta J)) / (1 - \exp(-2\beta J))]} \\ &\approx \frac{1}{\ln [(1 + \exp(-2\beta J)) (1 + \exp(-2\beta J))]} \quad \text{for } T \rightarrow 0^+ \\ &\approx \frac{1}{\ln [1 + 2\exp(-2\beta J)]} \quad \text{for } T \rightarrow 0^+ \\ &\rightarrow \frac{1}{2} \exp(2\beta J) \quad \text{for } T \rightarrow 0^+.\end{aligned}$$

$$\xi(T, 0) \rightarrow \begin{cases} 0 & \text{for } T \rightarrow \infty \\ \frac{1}{2} \exp(2\beta J) & \text{for } T \rightarrow 0^+ \\ 0 & \text{for } T = 0. \end{cases}$$



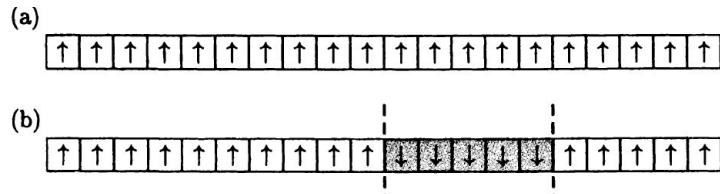
Critical temperature

We conclude our analysis of the one-dimensional Ising model by remarking on the role played by the temperature $T = 0$ in zero external field. Approaching this value, the susceptibility and the correlation length diverge.

This is intimately related to the onset of spontaneous magnetisation at $T = 0$. We can therefore identify the critical point $(T_c, H_c) = (0, 0)$, at which the phase transition takes place.

To investigate whether the single domain of aligned spins is stable against thermal fluctuations for $T > 0$, we calculate the difference between the free energy for a single domain of aligned spins, $F_{1\text{-dom}}$ and the free energy for two domains of oppositely aligned spins, $F_{2\text{-dom}}$.

We will show that for any finite temperature $T > 0$, $F_{2\text{-dom}} < F_{1\text{-dom}}$ when $N \rightarrow \infty$.



$$\begin{aligned}
 F_{2\text{-dom}} - F_{1\text{-dom}} &= -NJ + 4J - k_B T \ln 2N(N-1) + NJ + k_B T \ln 2 \\
 &= 4J - k_B T \ln N(N-1) \\
 &\approx 4J - 2k_B T \ln N \quad \text{for large } N.
 \end{aligned} \tag{2.96}$$

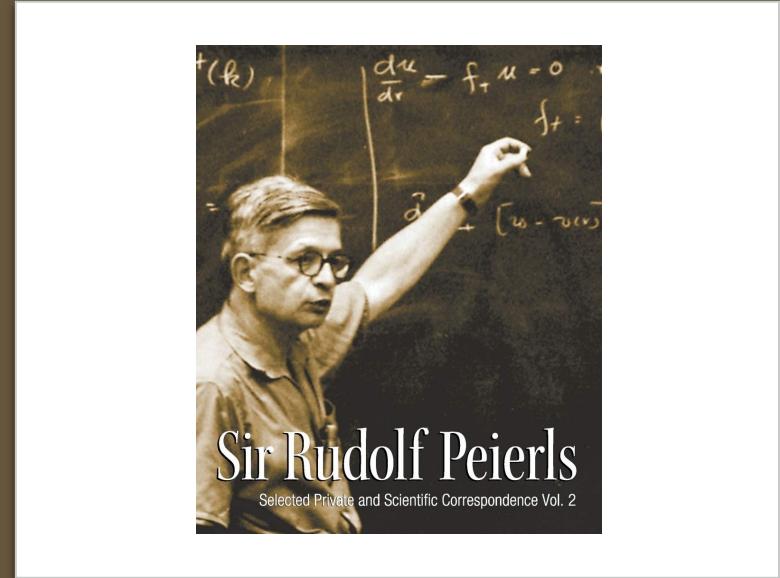
There are two microstates with a single spin domain, each with energy $-NJ$. The entropic contribution to the free energy is $-kT \ln 2$. Hence, the associated free energy for a single spin domain $F_{1\text{-dom}} = -NJ - kT \ln 2$.

To make two domains of oppositely aligned spins, two domain walls must be inserted with an energy cost of $4J$. There are $2N(N-1)$ equally probable microstates with two domain walls. The free energy is then $F_{2\text{-dom}} = -NJ + 4J - kT \ln 2N(N-1)$.

Peierls argument

Thus, for any finite temperature, it is energetically favourable to insert at least two domain walls when $N \rightarrow \infty$. However, the ensemble average over all these microstates gives zero magnetisation. Thus the critical temperature $T_c = 0$ for the one-dimensional Ising model.

In conclusion, there is no phase transition at any finite temperature in the one-dimensional Ising model.



Sir Rudolf Peierls

Selected Private and Scientific Correspondence Vol. 2

For large N

$$\frac{2J}{k_B T} < \ln N.$$

Mean-field theory for the Ising model

It is relatively easy to solve the Ising model analytically when ignoring fluctuations. Such an approach is generically referred to as mean field, and is often the first port of call when a non-trivial problem is encountered.

In order to explicitly expose where the fluctuations enter the Ising model, we first rewrite the interaction energy as follows:

$$\begin{aligned} E_{\text{int}} &= -J \sum_{\langle ij \rangle} s_i s_j \\ &= -J \sum_{\langle ij \rangle} (s_i - \langle s_i \rangle + \langle s_i \rangle)(s_j - \langle s_j \rangle + \langle s_j \rangle) \\ &= -J \sum_{\langle ij \rangle} [(s_i - \langle s_i \rangle)\langle s_j \rangle + (s_j - \langle s_j \rangle)\langle s_i \rangle + \langle s_i \rangle\langle s_j \rangle + (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle)]. \end{aligned} \tag{2.98}$$

When fluctuations around the average magnetisation per spin are small, we can neglect the second-order term. This in turn simplifies the problem by discounting spin-spin interactions.

Since the Ising model is translationally invariant, we can write the energy as

Therefore, the mean-field Ising model with coordination number z becomes a system of non-interacting spins immersed in an effective field of strength $(Jzm + H)$ plus a constant term $NJzm^2/2$. The effective field is made up of an 'internal' field, Jzm , resulting from the z nearest neighbours each contributing a field of strength Jm , and the external field H .

$$\begin{aligned} E_{\{s_i\}} &\approx -J \sum_{\langle ij \rangle} [(s_i + s_j)m - m^2] - H \sum_{i=1}^N s_i \\ &= -2Jm \sum_{\langle ij \rangle} s_i + J \sum_{\langle ij \rangle} m^2 - H \sum_{i=1}^N s_i \\ &= -2Jm \frac{z}{2} \sum_{i=1}^N s_i + J \frac{Nz}{2} m^2 - H \sum_{i=1}^N s_i \\ &= -(Jzm + H) \sum_{i=1}^N s_i + \frac{NJz}{2} m^2. \end{aligned}$$

The partition function is

$$\begin{aligned}
 Z &= \sum_{\{s_i\}} \exp \left((\beta J z m + \beta H) \sum_{i=1}^N s_i - \beta N J z m^2 / 2 \right) \\
 &= \exp (-\beta N J z m^2 / 2) \sum_{\{s_i\}} \prod_{i=1}^N \exp [(\beta J z m + \beta H) s_i] \\
 &= \exp (-\beta N J z m^2 / 2) [2 \cosh (\beta J z m + \beta H)]^N.
 \end{aligned}$$

And the free energy is

$$\begin{aligned}
 f &= -\frac{1}{N} k_B T \ln \left[\exp (-\beta N J z m^2 / 2) [2 \cosh (\beta J z m + \beta H)]^N \right] \\
 &= \frac{J z m^2}{2} - k_B T \ln [2 \cosh (\beta J z m + \beta H)]. \quad (1)
 \end{aligned}$$

To calculate the average magnetisation per spin m we keep in mind that it is a function of the temperature T , and the external field H .

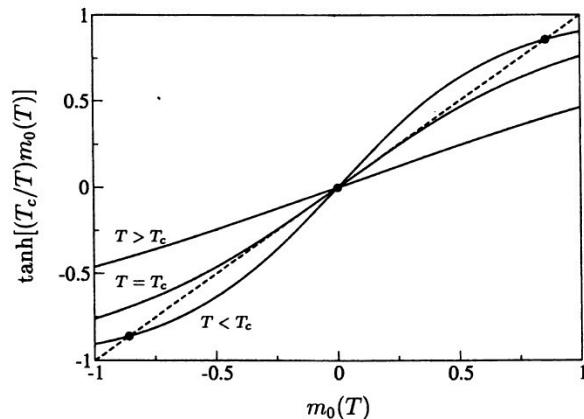
$$\begin{aligned}
 m &= - \left(\frac{\partial f}{\partial H} \right)_T \\
 &= -J z m \left(\frac{\partial m}{\partial H} \right)_T + k_B T \frac{2 \sinh(\beta J z m + \beta H)}{2 \cosh(\beta J z m + \beta H)} \left(\beta J z \left(\frac{\partial m}{\partial H} \right)_T + \beta \right) \\
 &= J z \left(\frac{\partial m}{\partial H} \right)_T [\tanh(\beta J z m + \beta H) - m] + \tanh(\beta J z m + \beta H). \quad (2.102)
 \end{aligned}$$

The average magnetization is then

$$m(T, H) = \tanh(\beta J z m + \beta H),$$

In zero field

$$m_0(T) = \tanh[\beta J z m_0(T)] = \tanh\left[\frac{T_c}{T} m_0(T)\right],$$



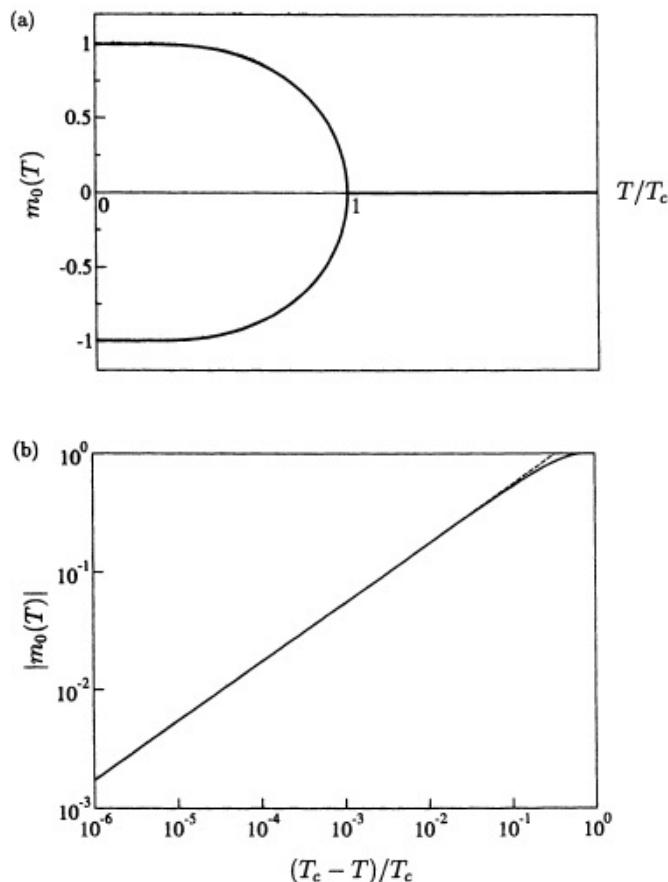
For all temperatures, $m_0(T) = 0$ is a solution. This solution is stable and unique for $T > T_c$, although only marginally so at $T = T_c$, and is unstable for $T < T_c$, where two stable non-zero solutions appear for the first time. Mean-field theory therefore predicts a phase transition at $T = T_c$ from a disordered phase with zero average magnetisation above T_c to an ordered phase with non-zero average magnetisation below T_c . The critical temperature for the mean-field theory of the Ising model is therefore $T_c = Jz/k_B$.

Magnetization in zero field

The average magnetisation per spin in zero external field, $m_0(T)$, versus the relative temperature T/T_c .

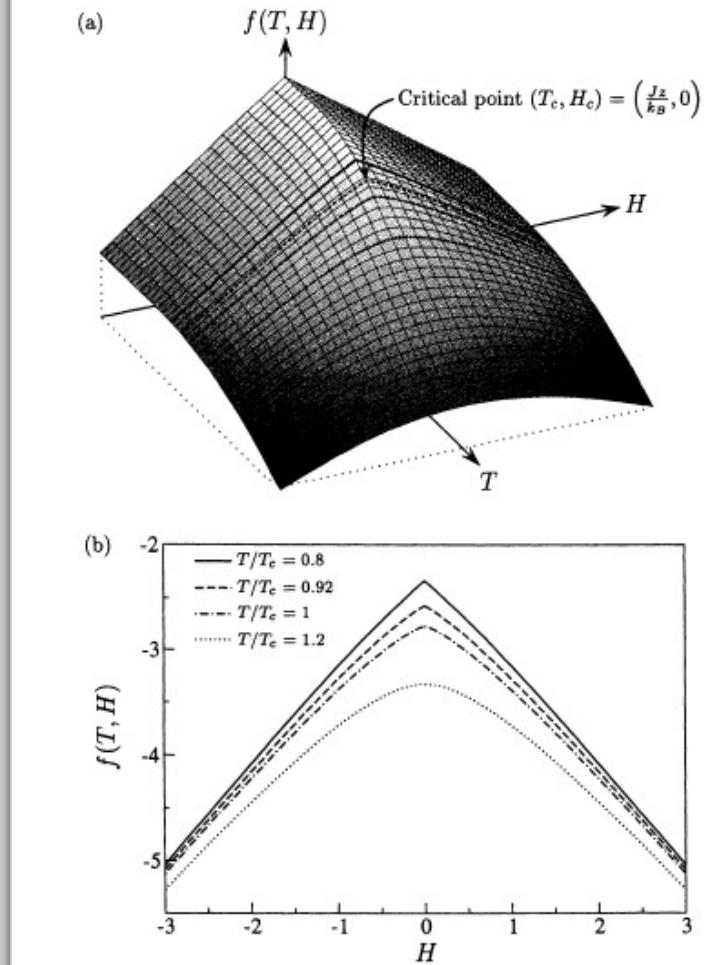
For $T > T_c$, $m_0(T) = 0$ but then picks up abruptly for $T < T_c$.

The absolute average magnetisation per spin in zero external field, $|m_0(T)|$, versus $(T_c - T)/T_c$ for $T < T_c$ (solid line). For $T < T_c$ the order parameter $m_0(T)$ prop $\pm(T_c - T)^\beta$ with $\beta = 1/2$. The dashed straight line has slope 1/2.



Free energy

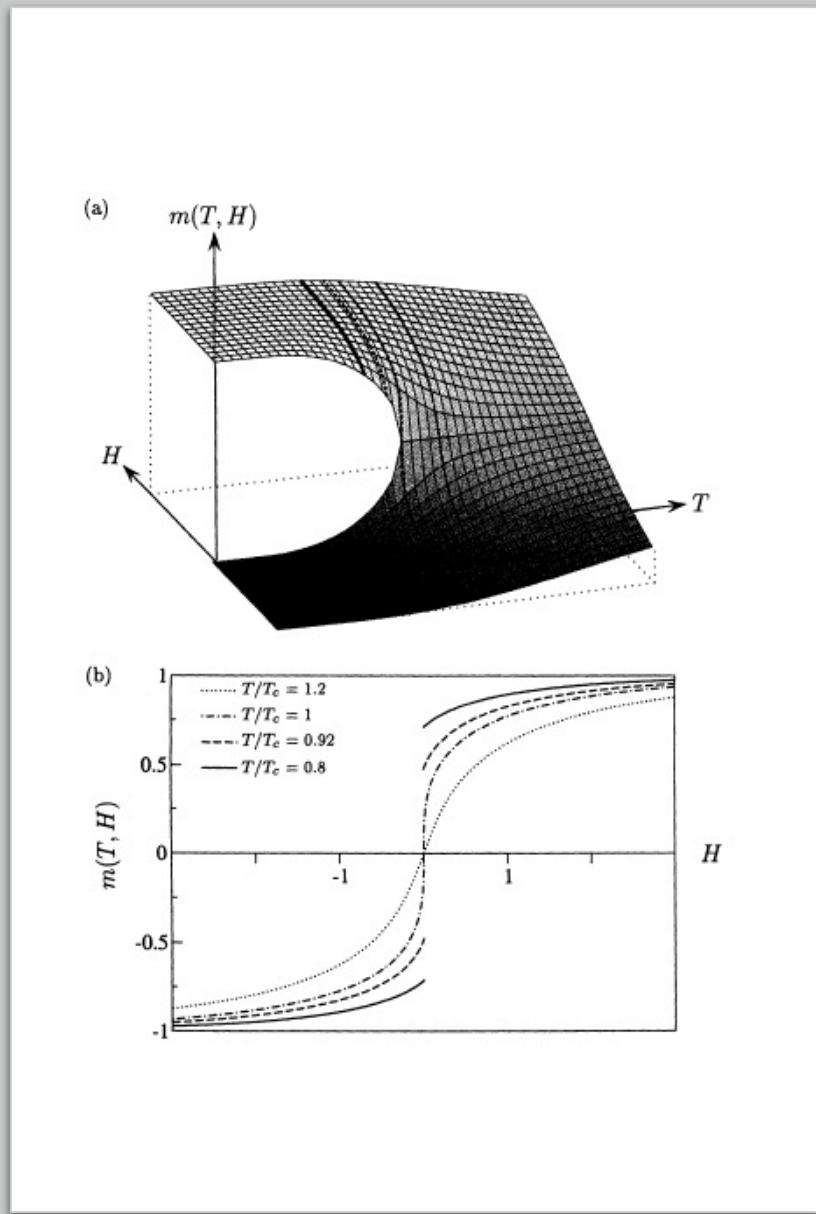
The free energy is analytic everywhere, except along the line $(T, 0)$ with $0 < T < T_c$, terminating at the critical point $(T_c, 0)$ where a cusp exists. Note that along the line $(T, 0)$ with $0 < T < T_c$, the left and right first derivatives of the free energy with respect to the external field are non-zero with opposite signs. This line of so-called first-order transitions ends at the critical point $(T_c, 0)$ where the first derivatives are zero.



Magnetization

The effect of the free energy per spin losing analyticity at the critical point is clearly visible, since, graphically, the magnetisation per spin is minus the slope of the free energy per spin as a function of external field for a given temperature.

Cut along the plane $H = 0$. For $T < T_c$, a discontinuous first-order phase transition occurs when switching the direction of the external field through $H = 0$. For $T = T_c$, the continuous second-order phase transition occurs, where the first derivative of the magnetisation per spin with respect to the external field diverges.



Magnetization

Expansion around T_c

To investigate the continuous but abrupt pick-up of the order parameter from zero average magnetisation, we expand the right-hand side of Equation (2.105) around $m_0(T) = 0$,

$$m_0(T) = \tanh\left[\frac{T_c}{T}m_0(T)\right] = \frac{T_c}{T}m_0(T) - \frac{1}{3}\left(\frac{T_c}{T}m_0(T)\right)^3 + \dots \quad (2.107)$$

Keeping the first two non-zero terms and rearranging,

$$m_0(T) \left[1 - \frac{T_c}{T} + \frac{1}{3}\left(\frac{T_c}{T}\right)^3 m_0^2(T)\right] = 0. \quad (2.108)$$

For $T < T_c$, the two non-trivial solutions are

$$m_0(T) = \pm\sqrt{3\left(\frac{T}{T_c}\right)^3}\sqrt{\frac{T_c - T}{T}} \quad \text{for } T \rightarrow T_c^-. \quad (2.109)$$

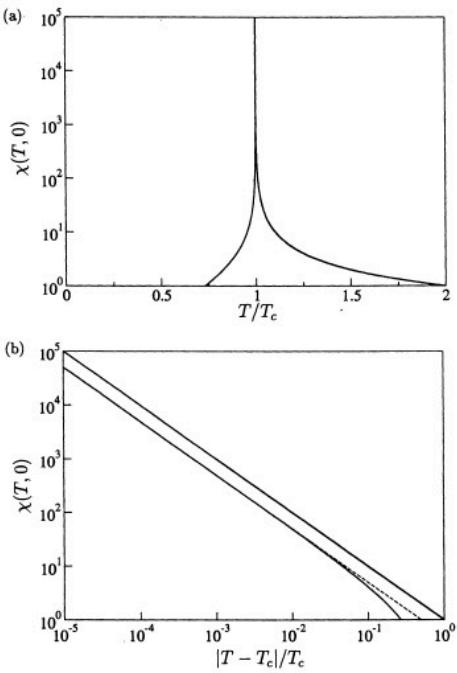
In summary, the order parameter

$$m_0(T) = \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\sqrt{3/T_c}(T_c - T)^\beta & \text{for } T \rightarrow T_c^- \end{cases}$$

where $\beta = 1/2$ for the mean-field theory of the Ising model.

Susceptibility

$$\left(\frac{\partial m}{\partial H}\right)_T = \operatorname{sech}^2\left(\frac{T_c}{T}m + \beta H\right) \left[\frac{T_c}{T} \left(\frac{\partial m}{\partial H}\right)_T + \beta \right].$$



To investigate how the susceptibility diverges as T approaches T_c in zero external field, we consider the two limits $T \rightarrow T_c^\pm$ separately, see Equation (2.110). When $T \rightarrow T_c^-$, the order parameter $m_0(T)$ approaches zero. Using the Taylor expansion $\cosh^2 x \approx 1 + x^2$, see Appendix A, we find

$$\begin{aligned} \chi(T, 0) &= \frac{1}{k_B} \frac{1}{T \cosh^2[(T_c/T)m_0(T)] - T_c} \\ &= \frac{1}{k_B} \frac{1}{T[1 + (T_c/T)^2 m_0^2(T)] - T_c} \\ &= \begin{cases} \frac{1}{k_B} (T - T_c)^{-\gamma^+} & \text{for } T > T_c \\ \frac{1}{2k_B} (T_c - T)^{-\gamma^-} & \text{for } T \rightarrow T_c^- . \end{cases} \end{aligned} \quad (2.113)$$

Hence, the susceptibility per spin in zero external field diverges as $T \rightarrow T_c^\pm$ as a power law with exponents γ^\pm in terms of the distance of T from T_c :

$$\chi(T, 0) \propto |T - T_c|^{-\gamma^\pm} \quad \text{for } T \rightarrow T_c^\pm, \quad (2.114)$$

see Figure 2.20(b). For the mean-field Ising model, $\gamma^\pm = 1$. We have explicitly demonstrated the general result that the critical exponents take the same value below and above T_c . In addition, the ratio of the amplitudes, Γ^\pm , which appear as prefactors in the power-law divergence, is universal,

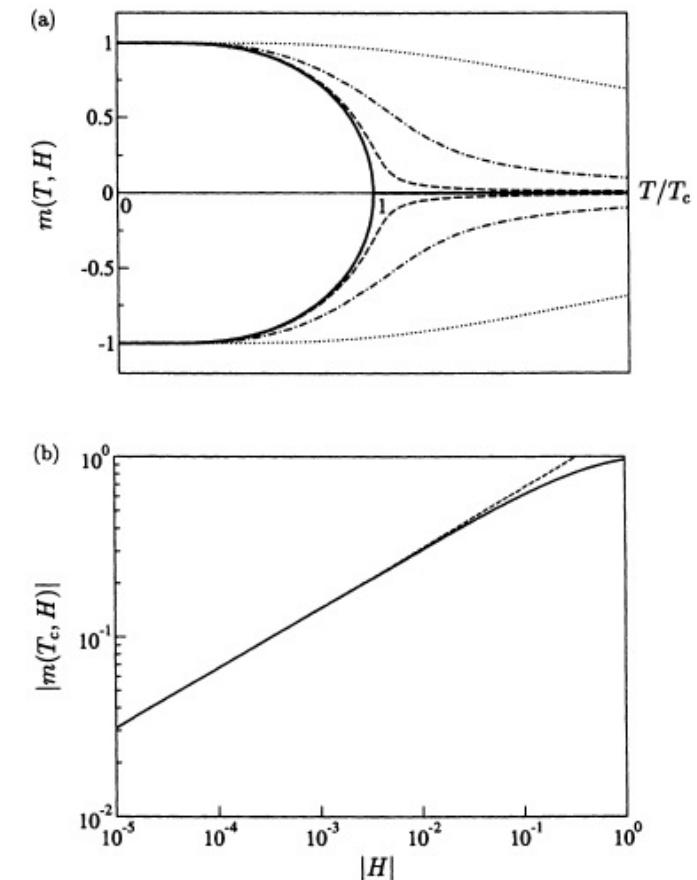
$$\frac{\Gamma^+}{\Gamma^-} = 2. \quad (2.115)$$

Magnetization in non-zero field

(a) displays the magnetisation per spin $m(T, H)$ versus the relative temperature T/T_c for various external fields. In the presence of a external field, the magnetisation becomes non-zero at $T = T_c$.

(b) displays the absolute average magnetisation per spin $|m(T_c, H)|$ at $T = T_c$ as a function of an applied positive external field.

Just as the critical exponent β describes the pick-up of the magnetisation in the vicinity of T_c - in zero external field, the critical exponent δ describes the magnetisation for small external fields at T_c .



Magnetization at Tc

We expand the right-hand side of Equation (2.104) at $T = T_c$ where $\beta_c J z = 1$ in a small external field, keeping terms to third order

$$\begin{aligned} m(T_c, H) &= \tanh(m + \beta_c H) \\ &= m + \beta_c H - \frac{1}{3}(m + \beta_c H)^3 + \dots \\ &= m + \beta_c H - \frac{1}{3}m^3 + \mathcal{O}(m^2 H, mH^2, H^3). \end{aligned} \quad (2.116)$$

After rearranging, we find that the mean-field Ising model predicts

$$m(T_c, H) = \text{sign}(H) (3\beta_c |H|)^{1/3} \propto \text{sign}(H) |H|^{1/\delta}, \quad (2.117)$$

with $\delta = 3$. Note that $m^2 H \propto m^5, mH^2 \propto m^7, H^3 \propto m^9$ so that Equation (2.116) is indeed an expansion to the third order in m . The dashed straight line in Figure 2.21(b) has slope $1/\delta = 1/3$.

Energy and specific heat

$$\begin{aligned}
 \varepsilon(T, 0) &= -\frac{1}{N} \frac{\partial \ln Z(T, 0)}{\partial \beta} \\
 &= \frac{Jz}{2} m_0^2(T) - \frac{2 \sinh[\beta J z m_0(T)]}{2 \cosh[\beta J z m_0(T)]} J z m_0(T) \\
 &= -\frac{Jz}{2} m_0^2(T) \\
 &= \begin{cases} 0 & \text{for } T \geq T_c \\ -\frac{3}{2} k_B(T_c - T) & \text{for } T \rightarrow T_c^- \end{cases},
 \end{aligned}$$

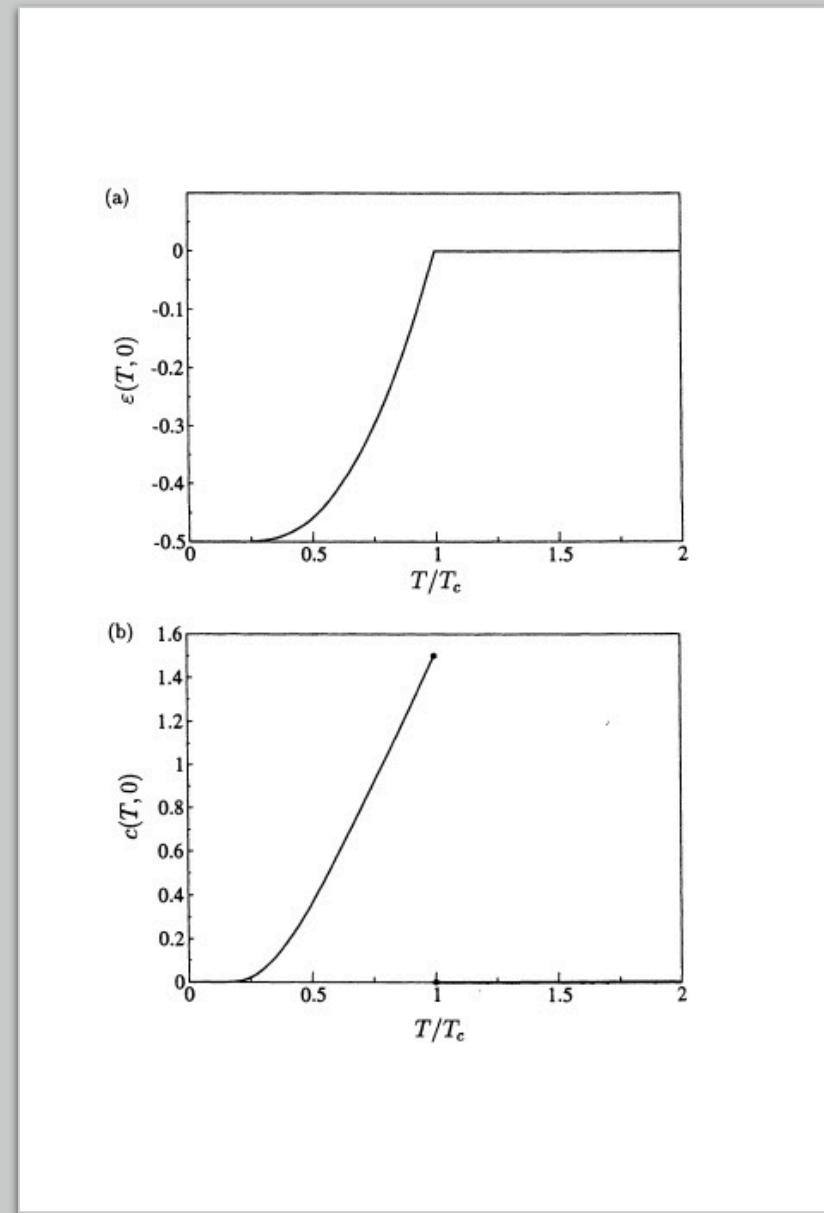
$$\begin{aligned}
 c(T, 0) &= \frac{\partial \varepsilon(T, 0)}{\partial T} \\
 &= k_B \left(\frac{T_c}{T} \right)^2 \frac{m_0^2(T)}{\cosh^2[(T_c/T)m_0(T)] - T_c/T} \\
 &= \begin{cases} 0 & \text{for } T \geq T_c \\ \frac{3}{2} k_B & \text{for } T \rightarrow T_c^- \end{cases}.
 \end{aligned}$$

The critical exponents α^\pm are defined through

$$c(T, 0) \propto |T - T_c|^{-\alpha^\pm} \quad \text{for } T \rightarrow T_c^\pm. \quad (2.120)$$

Therefore, we conclude that for the mean-field theory of the Ising model $\alpha^- = 0$. The critical exponent α^+ associated with the limit $T \rightarrow T_c^+$ is not defined in the simple mean-field treatment presented here. However, more elaborate mean-field approaches [Pathria, 1996] yield

$$\alpha^\pm = 0. \quad (2.121)$$



Summary

We summarise the success of mean-field theory for the Ising model. Most importantly, it predicts a second-order phase transition at a finite critical temperature and zero external field, which is correct for $d > 1$. There is also a line of first-order transitions $(T, 0)$ for $0 \leq T < T_c$ terminating at the critical point. The increase of the critical temperature $T_c = Jz/k_B$ with the coupling constant and the coordination number is qualitatively correct. Therefore, just as for percolation, the critical point depends on lattice details and is not a universal quantity. However, the critical exponents $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$ and $\delta = 3$ do not depend on the coupling constant and the coordination number and are indeed universal. Finally, mean-field theory predicts universal amplitude ratios, as in Equation (2.115).

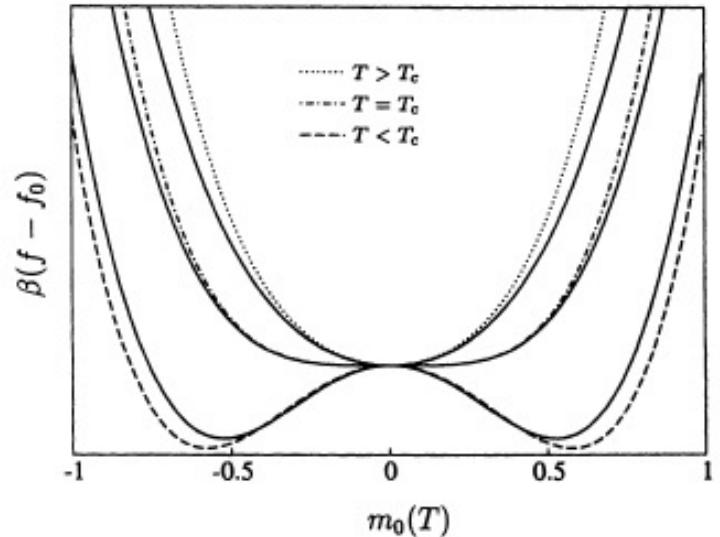
Landau theory for the Ising model

An alternative and more fundamental approach to characterising the minima of the free energy is to perform a Taylor expansion of the free energy itself in powers of the order parameter. Of course, such an expansion is only valid when the order parameter is small, that is, in the vicinity of the critical temperature and zero external field. To see how this works in practice, after introducing $f_0 = -k_B T \ln 2$ as the entropic (high temperature) part of the free energy per spin, Equation (2.101) becomes

$$f = f_0 + \frac{Jzm^2}{2} - k_B T \ln [\cosh (\beta Jzm + \beta H)]. \quad (2.124)$$

We now Taylor expand to fourth order the logarithmic term on the right-hand side of Equation (2.124) around $(T_c, 0)$ first using $\cosh x = 1 + x^2/2! + x^4/4! + \dots$ and then $\ln(1 + x) = x - x^2/2 + \dots$, see Appendix A, implying

$$\begin{aligned} \ln(\cosh x) &= \ln \left(1 + \frac{1}{2!}x^2 + \frac{1}{4!}x^4 + \dots \right) \\ &= \frac{1}{2!}x^2 + \frac{1}{4!}x^4 - \frac{1}{2} \left(\frac{1}{2!}x^2 + \frac{1}{4!}x^4 \right)^2 + \dots \\ &= \frac{1}{2}x^2 - \frac{1}{12}x^4 + \mathcal{O}(x^6). \end{aligned} \quad (2.125)$$



Substituting the expansion with $x = (T_c/T)m + \beta H$ into Equation (2.124) we find

$$f = f_0 + \frac{Jzm^2}{2} - k_B T \left[\frac{1}{2} \left(\frac{T_c}{T}m + \beta H \right)^2 - \frac{1}{12} \left(\frac{T_c}{T}m + \beta H \right)^4 \right]. \quad (2.126)$$

Collecting terms in increasing powers of m up to fourth order, the free energy becomes

$$f = f_0 - \frac{T_c}{T}Hm + \frac{1}{2}k_B \frac{T_c}{T}(T - T_c)m^2 + \frac{1}{12}k_B T \left(\frac{T_c}{T} \right)^4 m^4. \quad (2.127)$$

Since $H \propto m^3$, see Equation (2.117), we have dropped the terms proportional to H^2, Hm^3, H^2m^2, H^3m , and H^4 , which are all of higher order than m^4 . Therefore, in the vicinity of $(T_c, 0)$ where $T_c/T \rightarrow 1$, the free energy to fourth order in the magnetisation reduces to

$$\begin{aligned} f &= f_0 - Hm + \frac{1}{2}k_B(T - T_c)m^2 + \frac{1}{12}k_B T m^4 \\ &= f_0 - Hm + a_2(T - T_c)m^2 + a_4 m^4 \quad \text{for } (T, H) \rightarrow (T_c, 0), \end{aligned} \quad (2.128)$$

where

$$f_0 = -k_B T \ln 2, \quad (2.129a)$$

$$a_2 = \frac{1}{2}k_B, \quad (2.129b)$$

$$a_4 = \frac{1}{12}k_B T. \quad (2.129c)$$

Note that the sign of the coefficient of m depends on the direction of the external field. The coefficient of m^2 , namely $a_2(T - T_c)$, changes sign at $T = T_c$, while the coefficient of m^4 is positive. The average magnetisation per spin $m(T, H)$ is now determined by minimising the free energy in Equation (2.128).

The starting point for all calculations is the Taylor expanded free energy per spin

$$f = f_0 - Hm + a_2(T - T_c)m^2 + a_4m^4, \quad (2.130)$$

which is valid in the vicinity of the critical temperature and small external fields. Figure 2.24(a) displays the free energy per spin $f - f_0$ in zero external field versus m_0 .

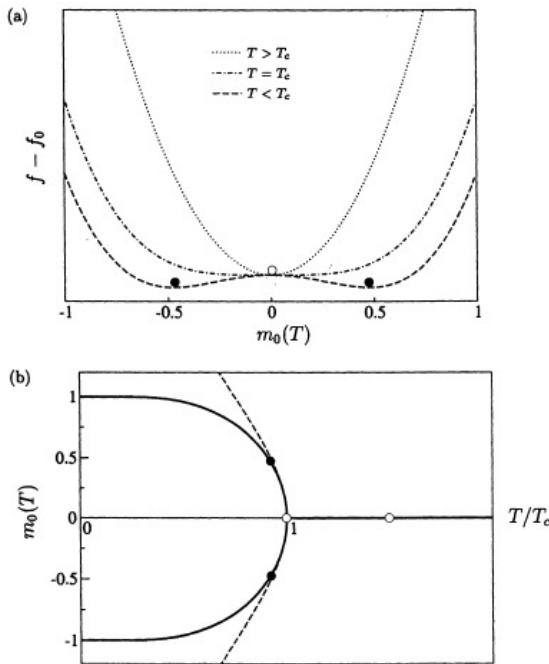
To find the average magnetisation per spin $m(T, H)$, we look for solutions of Equation (2.122),

$$-H + 2a_2(T - T_c)m + 4a_4m^3 = 0, \quad (2.131)$$

that minimise the free energy.

Magnetization

$$\beta = 1/2$$



In zero external field, Equation (2.131) reduces to

$$2m_0(T)[a_2(T - T_c) + 2a_4m_0^2(T)] = 0. \quad (2.132)$$

For all temperatures $m_0(T) = 0$ is a solution. When $T > T_c$, the square bracket is always positive so that the only solution is $m_0(T) = 0$. When $T = T_c$, the first term in the square bracket vanishes so that the only solution is $m_0(T) = 0$. However, when $T < T_c$, two additional solutions appear, $m_0(T) = \pm\sqrt{a_2(T_c - T)/2a_4}$. These two solutions minimise the free energy, see Figure 2.24(a).

In summary, the magnetisation per spin in zero external field,

$$\begin{aligned} m_0(T) &= \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\sqrt{a_2(T_c - T)/2a_4} & \text{for } T \rightarrow T_c^- \end{cases} \\ &= \begin{cases} 0 & \text{for } T \geq T_c \\ \pm\sqrt{3/T_c} (T_c - T)^\beta & \text{for } T \rightarrow T_c^- \end{cases}, \end{aligned} \quad (2.133)$$

Susceptibility in zero field

$$\gamma = 1$$

To determine the susceptibility per spin, we take the partial derivative of Equation (2.131) with respect to H ,

$$-1 + 2a_2(T - T_c) \left(\frac{\partial m}{\partial H} \right)_T + 12a_4m^2 \left(\frac{\partial m}{\partial H} \right)_T = 0. \quad (2.134)$$

To investigate how the susceptibility per spin diverges as T approaches T_c in zero external field, we solve Equation (2.134) for $(\partial m / \partial H)_T$ and substitute m with $m_0(T)$. Considering the two limits $T \rightarrow T_c^\pm$ separately, see Equation (2.133), we find

$$\begin{aligned} \chi(T, 0) &= 1/(2a_2(T - T_c) + 12a_4m_0^2) \\ &= \begin{cases} 1/2a_2(T - T_c) & \text{for } T \rightarrow T_c^+ \\ 1/[2a_2(T - T_c) + 12a_4(a_2(T_c - T)/2a_4)] & \text{for } T \rightarrow T_c^- \end{cases} \\ &= \begin{cases} \frac{1}{k_B}(T - T_c)^{-\gamma^+} & \text{for } T \rightarrow T_c^+ \\ \frac{1}{2k_B}(T_c - T)^{-\gamma^-} & \text{for } T \rightarrow T_c^-, \end{cases} \end{aligned} \quad (2.135)$$

(using $2a_2 = k_B$, see Equation (2.129b)) with the critical exponents $\gamma^\pm = 1$, in agreement with the mean-field results in Equation (2.113).

Magnetization at T_c

$$\delta = 3$$

To extract the critical exponent δ that describes the magnetisation for small external fields at T_c , we evaluate Equation (2.131) at T_c with the coefficients given in Equation (2.129) and find

$$-H + \frac{1}{3}k_B T_c m^3 = 0 \quad \text{for } T = T_c. \quad (2.136)$$

After rearranging, we recover the mean-field result of Equation (2.117)

$$m(T_c, H) = \text{sign}(H) (3\beta_c |H|)^{1/3} \propto \text{sign}(H) |H|^{1/\delta}, \quad (2.137)$$

with the critical exponent $\delta = 3$.

Specific heat

$$\alpha = 0$$

The specific heat is related to the second partial derivative of the free energy with respect to temperature. Therefore, we first substitute Equation (2.133) into Equation (2.130) to obtain the free energy per spin as a function of temperature,

$$\begin{aligned} f &= \begin{cases} f_0 & \text{for } T > T_c \\ f_0 + a_2(T - T_c)(a_2(T_c - T)/2a_4) + a_4a_2^2(T - T_c)^2/4a_4^2 & \text{for } T \rightarrow T_c^- \end{cases} \\ &= \begin{cases} f_0 & \text{for } T > T_c \\ f_0 - a_2^2(T - T_c)^2/4a_4 & \text{for } T \rightarrow T_c^- \end{cases} \\ &= \begin{cases} f_0 & \text{for } T > T_c \\ f_0 - \frac{3}{4T_c}k_B(T - T_c)^2 & \text{for } T \rightarrow T_c^- , \end{cases} \end{aligned} \quad (2.138)$$

such that the specific heat in zero external field is

$$c(T, 0) = -T \left(\frac{\partial^2 f}{\partial T^2} \right) \Big|_{H=0} = \begin{cases} 0 & \text{for } T > T_c \\ \frac{3}{2}k_B & \text{for } T \rightarrow T_c^- , \end{cases} \quad (2.139)$$

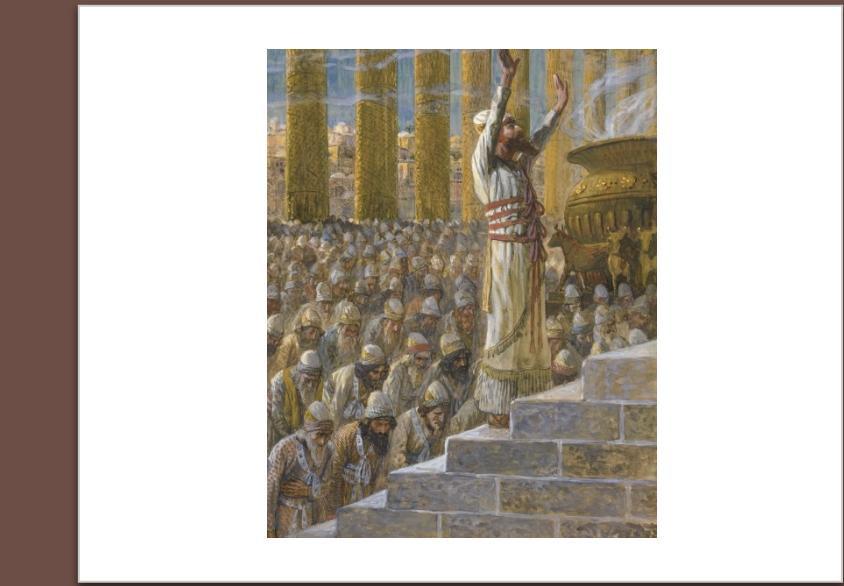
consistent with the results in Equation (2.119). Thus we recover the mean-field exponent $\alpha^- = 0$.

Biblical theory

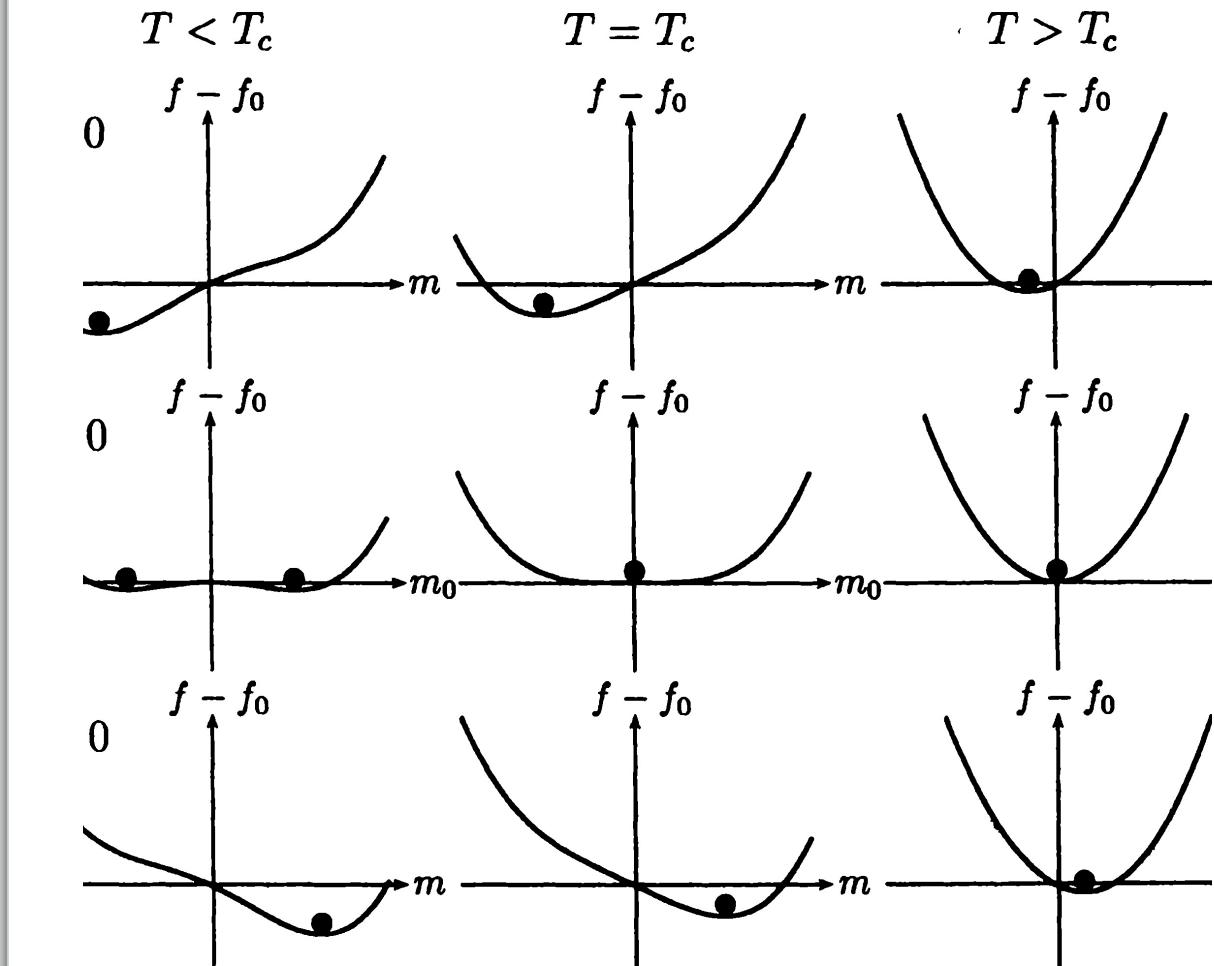
The Molten Sea or Brazen Sea was a large basin in the Temple for ablution of the priests. It is described in 1 Kings 7:23–26 and 2 Chronicles 4:2–5. It stood in the south-eastern corner of the inner court.

According to the Bible it was five cubits high, ten cubits in diameter from brim to brim, and thirty cubits in circumference.

$$\pi = 3$$



Landau Theory



Landau Theory

The Taylor expansion of the mean-field free energy is a specific example of a general phenomenological approach to continuous phase transitions devised by Landau in 1937 [Landau, 1937]. Landau was awarded the Nobel prize in physics 1962 for ‘his pioneering theories for condensed matter, especially liquid helium’ explaining the fluid-superfluid phase transition in ^4He . He argued that if the free energy is analytic near the critical point, then it can be expanded in terms of the order parameter which is small in the vicinity of the phase transition

$$f(T, H; \phi) = \sum_{k=0}^{\infty} \alpha_k(T, H) \phi^k \quad \text{for } T \rightarrow T_c, H \rightarrow 0, \quad (2.140)$$

where ϕ denotes a general order parameter and $\alpha_k(T, H)$ are coefficients that depend on the control parameters. For example, in the Ising model these control parameters are the temperature and the external field. We remind the reader that the order parameter is defined implicitly by minimising the free energy and is thus not an independent variable in the same way that the temperature and the external field are.

Landau theory

Symmetry arguments can be used to constrain the coefficients $\alpha_k(T, H)$. For example, for the Ising model in zero external field, the free energy is an even function of the order parameter, since in the absence of any external field the spins are equally likely to be pointing up or down, on average. This up-down symmetry is mathematically expressed as

$$f(T, 0; \phi) = f(T, 0; -\phi), \quad (2.141)$$

from which it immediately follows that no odd powers of ϕ may appear in Equation (2.140), so that $\alpha_k(T, 0) = 0$ for odd k in zero external field.

In the vicinity of the phase transition, the order parameter is small. Thus we expect the higher-order terms in the expansion of the free energy to be negligible. Furthermore, our experience with a mean-field Ising model leads us to expect three extrema for the free energy when $T < T_c$.

Therefore, in zero external field, the simplest possible form of the free energy that can describe a continuous phase transition is a fourth-order polynomial in even powers of the order parameter

$$f(T, 0; \phi) = \alpha_0(T, 0) + \alpha_2(T, 0)\phi_0^2 + \alpha_4(T, 0)\phi_0^4. \quad (2.142)$$

When $T > T_c$, the order parameter is zero and $\alpha_0(T, 0)$ is the only term remaining in the expansion of the free energy. Thus we identify $\alpha_0(T, 0)$ as the entropic part of the free energy since the average energy is zero.

Landau theory

Furthermore, the free energy has a unique extremum at $\phi_0 = 0$ which is a stable minimum. It follows that the coefficients $\alpha_2(T, 0)$ and $\alpha_4(T, 0)$ are positive for $T > T_c$.

When $T < T_c$, the order parameter is non-zero and all three terms are present in the expansion of the free energy. The free energy has three extrema, one unstable maximum at zero order parameter, and two stable minima at non-zero order parameters, symmetric around zero. It follows that the coefficient $\alpha_2(T, 0)$ is negative and $\alpha_4(T, 0)$ is positive for $T < T_c$.

At $T = T_c$, the free energy has a unique extremum at $\phi_0 = 0$ which is a marginally stable minimum. Since $\alpha_2(T, 0)$ is positive for $T > T_c$ and negative for $T < T_c$, it follows that $\alpha_2(T, 0)$ must be zero at $T = T_c$. However, $\alpha_4(T, 0)$ remains positive to ensure that the extremum is a minimum.

Assuming that the coefficients $\alpha_k(T, H)$ are analytic around $(T_c, 0)$, they can themselves be expanded in powers of $(T - T_c)$ and H . For temperatures close to the critical temperature and small external fields, it is sufficient to keep only the leading-order term.

The leading-order terms for $\alpha_0(T, H)$ and $\alpha_4(T, H)$ are the zeroth-order terms $\tilde{\alpha}_0$, for which the sign is irrelevant, and $\tilde{\alpha}_4$, which is positive.

The leading-order term for $\alpha_2(T, H)$ is the first-order term,

$$\alpha_2(T, H) = \tilde{\alpha}_2(T - T_c) \quad \text{for } T \rightarrow T_c, H \rightarrow 0, \quad (2.143)$$

where $\tilde{\alpha}_2$ is positive.

If we restore a small external field, the coefficients $\alpha_k(T, H)$ with odd k become non-zero. The leading-order term for $\alpha_1(T, H)$ is the first-order term

$$\alpha_1(T, H) = \tilde{\alpha}_1 H \quad \text{for } T \rightarrow T_c, H \rightarrow 0. \quad (2.144)$$

Summary

In summary, in the Landau theory of continuous (second-order) phase transitions with order parameter ϕ , the simplest form of the free energy is

$$f(T, H; \phi) = \bar{\alpha}_0 + \bar{\alpha}_1 H\phi + \bar{\alpha}_2(T - T_c)\phi^2 + \bar{\alpha}_4\phi^4, \quad (2.145)$$

where $\bar{\alpha}_0$ is the entropic part of the free energy, $\bar{\alpha}_1 = -1$, $\bar{\alpha}_2 > 0$, and the coefficient of ϕ^2 changes sign at T_c , and $\bar{\alpha}_4 > 0$. The coefficients in Equation (2.128) are consistent with the general considerations of the phenomenological Landau theory of continuous phase transitions.

Following the steps in Sections 2.6.2 and 2.6.3 one could once again derive the mean-field exponents for the Ising model, $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$, and $\delta = 3$.



Landau Theory

Most phases can be understood through the lens of spontaneous symmetry breaking. For example, crystals are periodic arrays of atoms that are not invariant under all translations (only under a small subset of translations by a lattice vector). Magnets have north and south poles that are oriented in a specific direction, breaking rotational symmetry. In addition to these examples, there are a whole host of other symmetry-breaking phases of matter — including nematic phases of liquid crystals, and many others in soft matter and beyond.

Lev Landau introduced a framework in an attempt to formulate a general theory of continuous (i.e., second-order) phase transitions. This theory can be extended to systems under externally-applied fields and used as a quantitative model for discontinuous (i.e., first-order) transitions.

Other generalizations include vector and tensor order parameters, appropriate to describe polar and nematic ordered phases. More complicated ordered phases, with two or more coupled order parameters may also be considered, and the generalized Landau theory is a useful tool to understand the structure of complex soft matter phases.

Scale invariance

In statistical mechanics, scale invariance is a feature of phase transitions. The key observation is that near a phase transition or critical point, fluctuations occur at all length scales, and thus one should look for an explicitly scale-invariant theory to describe the phenomena. Such theories are scale-invariant statistical field theories, and are formally very similar to scale-invariant quantum field theories.



Widom scaling ansatz

The failure of mean-field theory in low dimensions motivates its replacement with a more general framework. Just as for the cluster number density in percolation, we now search for a general scaling ansatz for the free energy per spin that compactly summarises the behaviour of the Ising model in the vicinity of the critical point. With a scaling ansatz for the free energy per spin, we would be able to derive a scaling ansatz for all thermodynamic quantities and establish scaling relations among the critical exponents.

It is convenient to introduce the dimensionless reduced temperature, t , and the dimensionless reduced external field, h :

$$t = \frac{T - T_c}{T_c}, \quad (2.162a)$$

$$h = \frac{H}{k_B T} = \beta H, \quad (2.162b)$$

such that the limits

$$t \rightarrow 0^\pm \Leftrightarrow T \rightarrow T_c^\pm, \quad (2.163a)$$

$$h \rightarrow 0^\pm \Leftrightarrow H \rightarrow 0^\pm. \quad (2.163b)$$

Widom scaling ansatz

The free energy $f(t, h)$ describes a two-dimensional surface which is analytic everywhere except along a line $(t, 0)$ for $-1 \leq t \leq 0$, terminating at the critical point $(0, 0)$ where a cusp exists, see e.g. Figure 2.18. The free energy can be decomposed into regular (analytic) and singular (non-analytic) parts, $f(t, h) = f_r(t, h) + f_s(t, h)$, and it is the latter that is responsible for the cusp. Since we are interested in the critical behaviour of the Ising model we are only concerned with the singular part of the free energy which contains information about critical exponents, scaling functions, associated amplitudes, and so on. Specifically, it is the singular part of the free energy $f_s(t, h)$ for which we construct the scaling ansatz.

We are more familiar with the behaviour of the magnetisation in the vicinity of the critical point; therefore we first discuss how to encapsulate its limiting behaviour in a compact scaling ansatz. Since the magnetisation is a partial derivative of the free energy with respect to the external field, we are then in a position to propose a scaling ansatz for the free energy.

Widom scaling ansatz

Recall that the magnetisation is an odd function of the external field

$$m(t, h) = -m(t, -h). \quad (2.164a)$$

In addition, the magnetisation per spin in the limit of zero external field

$$\lim_{h \rightarrow 0^\pm} m(t, h) \propto \begin{cases} 0 & \text{for } t \geq 0 \\ \pm|t|^\beta & \text{for } t \rightarrow 0^-, \end{cases} \quad (2.164b)$$

and for small external fields at $t = 0$

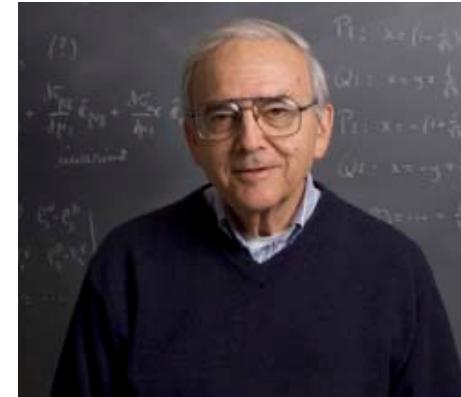
$$m(0, h) \propto \text{sign}(h)|h|^{1/\delta} \quad \text{for } h \rightarrow 0^\pm. \quad (2.164c)$$

The symmetry and the limiting behaviours can be compactly summarised in the following Widom scaling ansatz for the magnetisation [Widom, 1965]:

$$m(t, h) = |t|^\beta \mathcal{M}_\pm(h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0, \quad (2.165)$$

where Δ is known as the gap exponent and \mathcal{M}_+ and \mathcal{M}_- are the scaling functions for the magnetisation per spin in the two regimes $t > 0$ and $t < 0$, respectively. Note that while the magnetisation per spin on the left-hand side of Equation (2.165) is a function of the reduced temperature t and the reduced external field h , the scaling functions on the right-hand side is only a function of the ratio $h/|t|^\Delta$.

Scaling of the magnetization



To recover the known behaviour of the magnetisation per spin in Equations (2.164), the scaling functions \mathcal{M}_\pm must satisfy certain constraints and the gap exponent Δ must be related to known exponents.

By symmetry, the scaling functions are odd functions

$$\mathcal{M}_\pm(x) = -\mathcal{M}_\pm(-x), \quad (2.166a)$$

and in the limit of zero external field

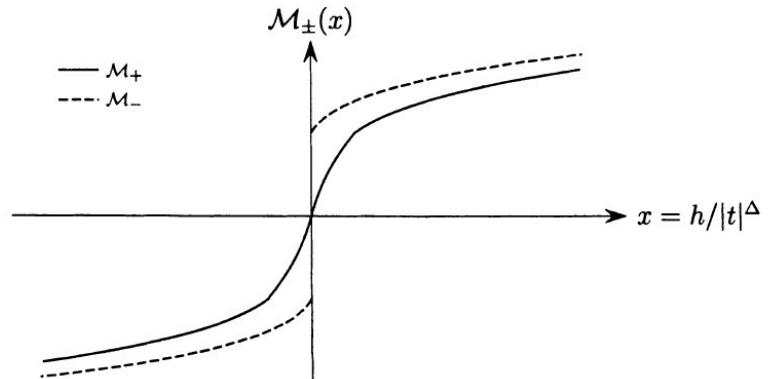
$$\begin{aligned} \lim_{x \rightarrow 0^\pm} \mathcal{M}_+(x) &= 0, \\ \lim_{x \rightarrow 0^\pm} \mathcal{M}_-(x) &= \pm \text{non-zero constant}. \end{aligned} \quad (2.166b)$$

Finally, when $t \rightarrow 0$ in small external field, the argument of the scaling functions $x = h/|t|^\Delta \rightarrow \pm\infty$. Therefore, we require

$$\begin{aligned} \mathcal{M}_\pm(x) &\propto \text{sign}(x)|x|^{1/\delta} \quad \text{for } x \rightarrow \pm\infty, \\ \Delta &= \beta\delta, \end{aligned} \quad (2.166c)$$

to ensure that

$$\begin{aligned} m(t, h) &\propto |t|^\beta \text{sign}(h) \left(|h|/|t|^\Delta\right)^{1/\delta} \quad \text{for } h \rightarrow 0^\pm, h/|t|^\Delta \rightarrow \pm\infty \\ &\propto \text{sign}(h)|h|^{1/\delta} \quad \text{for } h \rightarrow 0^\pm, h/|t|^\Delta \rightarrow \pm\infty. \end{aligned} \quad (2.167)$$



Scaling for the free energy and the specific heat

We now propose a scaling ansatz for the singular part of the free energy per spin which must be consistent with the magnetisation per spin in Equation (2.165), and the singular behaviour of the susceptibility per spin and the specific heat. Widom argued that

$$f_s(t, h) = |t|^{2-\alpha} \mathcal{F}_\pm(h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0, \quad (2.168)$$

where \mathcal{F}_+ and \mathcal{F}_- are the scaling functions for the free energy per spin in the two regimes $t > 0$ and $t < 0$, respectively [Widom, 1965]. Note that while the free energy on the left-hand side of Equation (2.168) is a function of the reduced temperature and the reduced external field, the scaling function on the right-hand side is only a function of the ratio $h/|t|^\Delta$. In Section 2.15 we will justify the Widom scaling ansatz by exploiting scale invariance at the critical point within the real-space renormalisation group theory.

Since we have the operator identity

$$\frac{\partial}{\partial T} = \frac{1}{T_c} \frac{\partial}{\partial t}, \quad (2.169)$$

we find for the specific heat,

$$\begin{aligned} c(t, h) &= -T \frac{1}{T_c^2} \left(\frac{\partial^2 f_s}{\partial t^2} \right)_h \\ &= -\frac{T}{T_c} \frac{(2-\alpha)(1-\alpha)}{T_c} |t|^{-\alpha} \mathcal{F}_\pm(h/|t|^\Delta) + \mathcal{O}(h, h^2) \\ &= |t|^{-\alpha} \mathcal{C}_\pm(h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0, \end{aligned} \quad (2.170)$$

where the scaling functions for the specific heat is given by

$$\mathcal{C}_\pm(x) = -\frac{(2-\alpha)(1-\alpha)}{T_c} \mathcal{F}_\pm(x). \quad (2.171)$$

In the limit of zero external field

$$c(t, 0) = |t|^{-\alpha} \mathcal{C}_\pm(0) \quad \text{for } t \rightarrow 0^\pm. \quad (2.172)$$

This explains why the exponent $2 - \alpha$ appears in the scaling ansatz for the free energy in Equation (2.168).

Widom scaling relation

To confirm that Equation (2.168) does contain the correct scaling ansatz for the magnetisation, we differentiate with respect to the external field H at fixed temperature. Using the operator identity

$$\frac{\partial}{\partial H} = \frac{1}{k_B T} \frac{\partial}{\partial h}, \quad (2.173)$$

we find for the magnetisation per spin,

$$\begin{aligned} m(t, h) &= -\frac{1}{k_B T} \left(\frac{\partial f_s}{\partial h} \right)_t \\ &= -\frac{1}{k_B T} |t|^{2-\alpha-\Delta} \mathcal{F}'_{\pm}(h/|t|^{\Delta}) \\ &= |t|^{2-\alpha-\Delta} \mathcal{M}_{\pm}(h/|t|^{\Delta}) \quad \text{for } t \rightarrow 0^{\pm}, h \rightarrow 0, \end{aligned} \quad (2.174)$$

where the scaling functions for the magnetisation per spin is given by

$$\mathcal{M}_{\pm}(x) = -\frac{1}{k_B T} \mathcal{F}'_{\pm}(x). \quad (2.175)$$

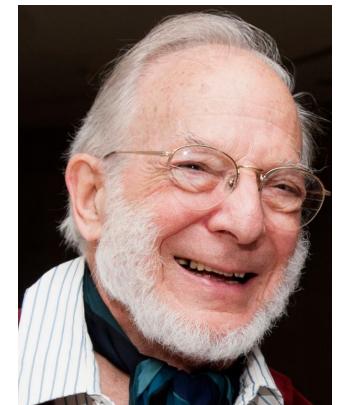
Taking the limit of zero external field,

$$\lim_{h \rightarrow 0^{\pm}} m(t, h) = |t|^{2-\alpha-\Delta} \lim_{x \rightarrow 0^{\pm}} \mathcal{M}_{\pm}(x) \propto \begin{cases} 0 & \text{for } t \rightarrow 0^+ \\ \pm |t|^{2-\alpha-\Delta} & \text{for } t \rightarrow 0^- \end{cases} \quad (2.176)$$

and we identify the scaling relation

$$2 - \alpha - \Delta = \beta. \quad (2.177)$$

Scaling for the susceptibility and correlation function



Using the operator identity in Equation (2.173), the susceptibility per spin

$$\begin{aligned}\chi(t, h) &= \frac{1}{k_B T} \left(\frac{\partial m}{\partial h} \right)_t \\ &= -\frac{1}{k_B^2 T^2} |t|^{2-\alpha-2\Delta} \mathcal{F}_\pm''(h/|t|^\Delta) \\ &= |t|^{2-\alpha-2\Delta} \chi_\pm(h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0,\end{aligned}\quad (2.178)$$

where the scaling functions for the susceptibility per spin is given by

$$\chi_\pm(x) = -\frac{1}{k_B^2 T^2} \mathcal{F}_\pm''(x). \quad (2.179)$$

Taking the limit of zero external field,

$$\chi(t, 0) = |t|^{2-\alpha-2\Delta} \chi_\pm(0), \quad (2.180)$$

and we conclude that

$$\begin{aligned}\chi_\pm(0) &= \text{non-zero constants}, \\ 2 - \alpha - 2\Delta &= -\gamma.\end{aligned}\quad (2.181)$$

Correlation function (Fisher)

$$g(r, t, h) \propto r^{-(d-2+\eta)} \mathcal{G}_\pm(r/\xi, h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0,$$

$$g(r, t, 0) \propto r^{-(d-2+\eta)} \mathcal{G}_\pm(r/\xi, 0) \quad \text{for } t \rightarrow 0^\pm.$$

$$\mathcal{G}_\pm(r/\xi, 0) \propto \begin{cases} \text{constant} & \text{for } r \ll \xi \\ (r/\xi)^{\eta+(d-3)/2} \exp(-r/\xi) & \text{for } r \gg \xi. \end{cases}$$

Scaling relations and hyperscaling

We note that the critical exponents are not independent. The divergences of the specific heat and the susceptibility in zero external field $h = 0$ as $t \rightarrow 0$ are described by α and γ , respectively. The pick-up of the order parameter $m(t, 0)$ at $t = 0$ is described by β , while δ describes how the order parameter $m(0, h)$ vanishes when the external field $h \rightarrow 0$. Finally, η is related to the power-law decay of the spin-spin correlation function at the critical point, while ν describes the divergence of the correlation length in zero external field as $t \rightarrow 0$. The critical exponents α, β, γ , and δ are a feature of the non-analyticity of the free energy at the critical point and are characterised by the geometry of the free energy surface in the vicinity of the cusp; they are therefore related through scaling relations.

Combining Equations (2.166c), (2.177) and (2.181) and eliminating Δ yields two scaling relations, namely

$$\beta\delta = \beta + \gamma, \quad (2.185)$$

$$\alpha + 2\beta + \gamma = 2. \quad (2.186)$$

Using a simple scaling argument, a third scaling relation follows from considering the singular part of free energy per spin in zero external field

$$f_s(t, 0) \propto |t|^{2-\alpha} \quad \text{for } t \rightarrow 0. \quad (2.187)$$

The free energy per spin is the density of the free energy and therefore scales with inverse volume⁷

$$f_s(t, 0) \propto L^{-d}, \quad (2.188)$$

so that the free energy density within a length scale ξ

$$f_s(t, 0) \propto \xi^{-d} \propto |t|^{\nu d} \quad \text{for } t \rightarrow 0. \quad (2.189)$$

Therefore, we conclude that

$$2 - \alpha = \nu d. \quad (2.190)$$

Summary

In summary, only two of the six critical exponents are independent since they obey the four scaling relations

$$\beta\delta = \beta + \gamma, \tag{2.195a}$$

$$\alpha + 2\beta + \gamma = 2, \tag{2.195b}$$

$$\gamma = \nu(2 - \eta), \tag{2.195c}$$

$$2 - \alpha = \nu d \quad \text{for } d \leq 4. \tag{2.195d}$$

Note that the first three relations are valid in all dimensions. The hyper-scaling relation in Equation (2.195d) involving the dimensionality is only valid for $d \leq 4$.

Critical temperatures



Table 2.3 The critical temperature in zero external field, $k_B T_c/J$, in units of J for various lattice types and dimensions in the Ising model. The second column lists the coordination number, z , for a given lattice.

Lattice	z	$k_B T_c/J$
$d = 1$ line	2	0
$d = 2$ hexagonal	3	$2/\ln(2 + \sqrt{3})^a$
square	4	$2/\ln(1 + \sqrt{2})^b \approx 2.269185$
triangular	6	$4/\ln 3^a$
$d = 3$ diamond	4	2.70^c
simple cubic	6	4.51152^d
body-centred cubic	8	6.40^e
face-centred cubic	12	9.79^e
Mean-field	z	z

^a[Baxter, 1982].

^b[Kramers and Wannier, 1941].

^c[Gaunt and Sykes, 1973].

^d[Arisue *et al.*, 2004].

^e[Sykes *et al.*, 1972].

Critical exponents



Table 2.4 The values of the critical exponents for the Ising model in dimensions $d = 1, 2, 3$, and $d \geq 4$, and in the mean-field theory of the Ising model. The critical exponents in $d = 3$ are not known exactly but the current best numerical results are listed with the uncertainty on the last digit(s) given by the figure(s) in the brackets. Two of the critical exponents have been measured numerically and the remaining critical exponents are evaluated from the scaling relations in Equation (2.195).

Exponent: Quantity	$d = 1^a$	$d = 2$	$d = 3$	$d \geq 4$	Mean-field
$\alpha : c(t, 0) \propto t ^{-\alpha}$	$2 - 2/k$	$0 (\log)$	$0.111(2)$	0	$0 (\text{dis})$
$\beta : m(t, 0) \propto (-t)^\beta$	0	$1/8$	$0.3262(13)^b$	$1/2$	$1/2$
$\gamma : \chi(t, 0) \propto t ^{-\gamma}$	$2/k$	$7/4$	$1.237(3)$	1	1
$\delta : m(0, h) \propto \text{sign}(h) h ^{1/\delta}$	∞	15	$4.792(18)$	3	3
$\nu : \xi(t, 0) \propto t ^{-\nu}$	$2/k$	1	$0.6297(8)^b$	$1/2$	$1/2$
$\eta : g(r, t, 0) \propto r^{-(d-2+\eta)} G_\pm(r/\xi, 0)$	1	$1/4$	$0.036(5)$	0	0

^aUsing the reduced ‘temperature’ $t = \exp(-kJ/k_B T)$, where $k > 0$ is a constant.

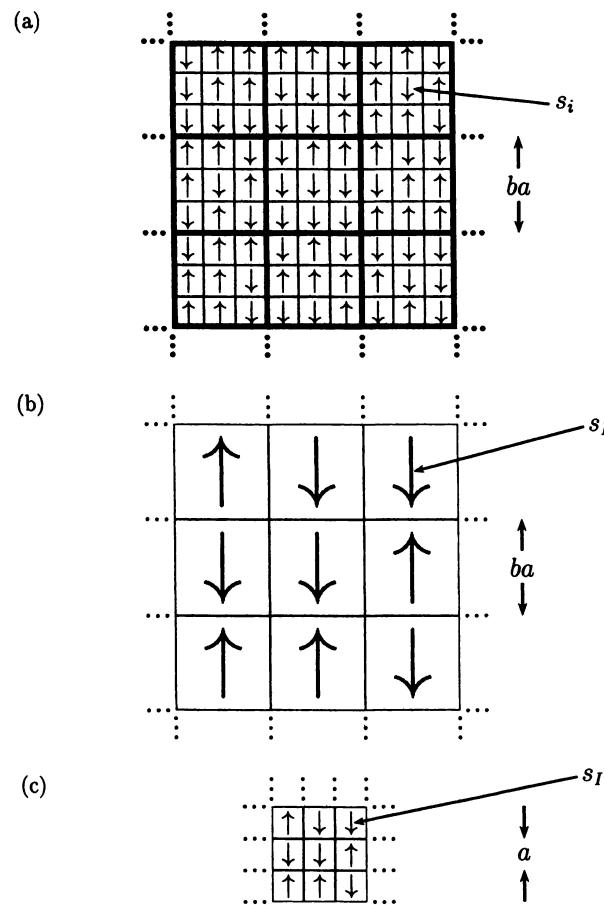
^b[Binder and Luijten, 2001].



Block spins

Kadanoff argued that since spins are correlated over scales up to the correlation length, it may be plausible to regard spins within regions up to ξ in size as-behaving like a single block spin [Kadanoff, 1966]. In this spirit, Kadanoff outlined a real-space renormalisation procedure over scales $b \leq \xi$

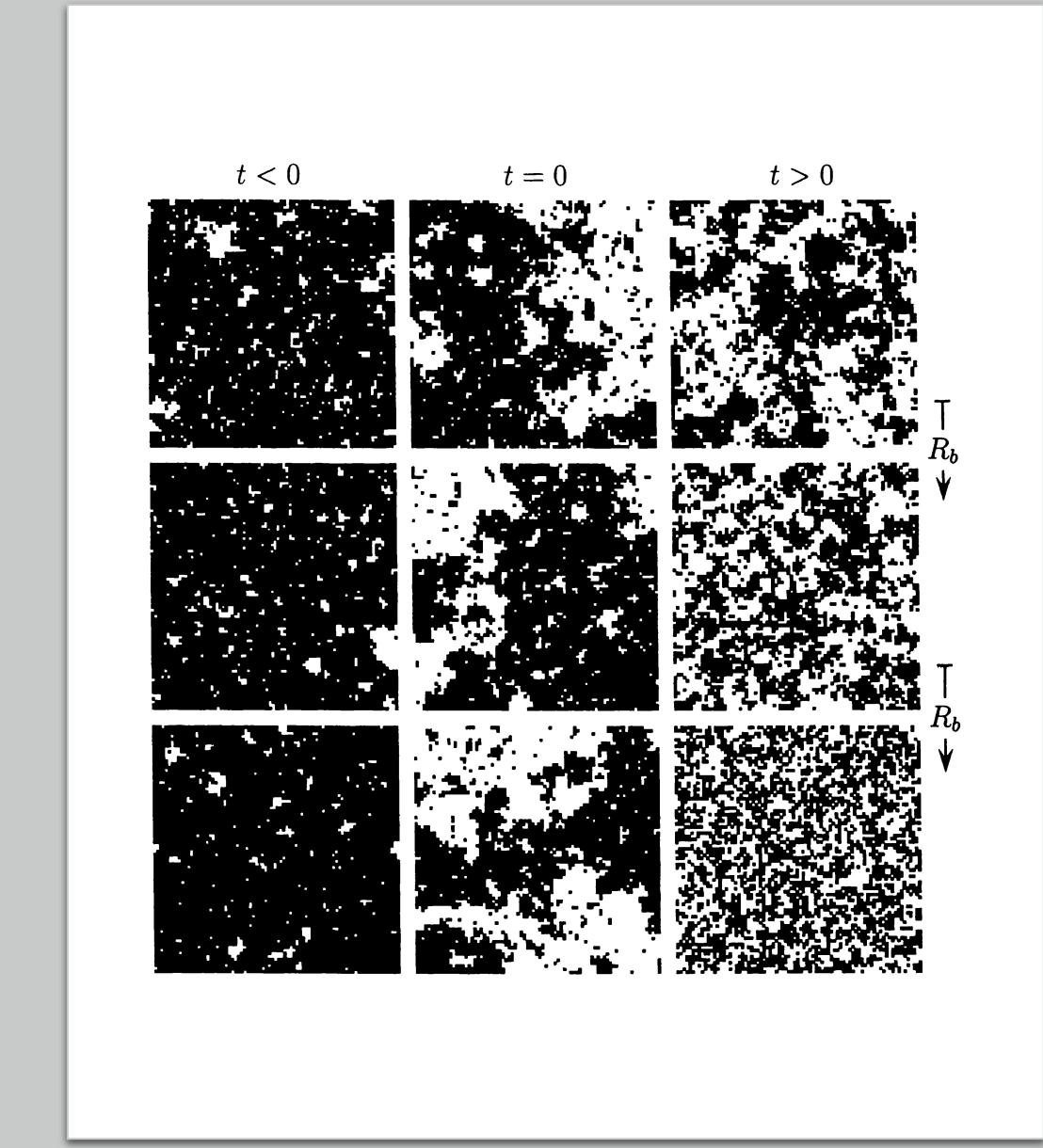
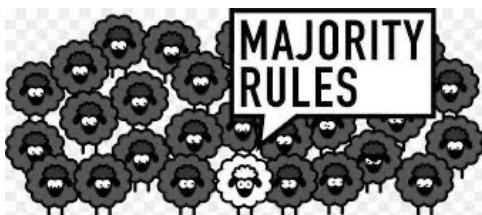
- (1) Divide the lattice into blocks, I , of linear size b (in terms of the lattice constant) with each block containing b^d spins, (a).
- (2) Replace each block I of spins with a single block spin, s_I , according to some coarse graining rule which is some function of the spins within block I , (b).
- (3) Rescale all lengths by the dimensionless scale factor b to restore the original lattice spacing



Coarse graining

Real-space renormalisation group transformation of the two-dimensional Ising model on a square lattice. The panels are windows of size $l = 80$ inside larger lattices.

The three panels in the top row correspond to lattices in zero external field with reduced temperatures $t < 0$, $t = 0$, $t > 0$ from left to right. In each of the three columns, the renormalisation transformation, R_b , is carried out twice from top to bottom, revealing large scale behaviour. Coarsening is achieved by employing the majority rule with $b = 3$.



Real space RG: correlation length

The real-space renormalisation reduces all lengths, including the correlation length, by a factor b . If the system is not at the critical point, the correlation length is finite and becomes shorter with each application of the renormalisation transformation. The reduction in the correlation length is associated with a flow away from the critical point. In terms of the reduced variables (t, h) , which gives the distance from the critical point, the flow can be described as $(t, h) \mapsto (t', h')$. If the system is at the critical point, the correlation length is infinite and is therefore unaffected by the renormalisation transformation. From the flow in the vicinity of the critical point, we note that if $t = 0$, $t' = 0$, while if $t > 0$, $t' > t$, and finally if $t < 0$, $t' < t$. Since the flow is directed away from the critical point, we deduce that $t' \propto t$, to first order. Similarly, by symmetry one can argue that $h' \propto h$, to first order.

Therefore, in the vicinity of the critical point, to first order, $t' = \lambda_t(b)t$ where $\lambda_t(b)$ is a proportionality constant that depends on the block size b . If $b > 1$, then $\lambda_t(b) > 1$ while $\lambda_t(1) = 1$. Renormalising twice with blocks of sizes b_1 and b_2 should be equivalent to renormalising once with a block

of size $b_1 b_2$. Therefore, $t'' = \lambda_t(b_2)t' = \lambda_t(b_2)\lambda_t(b_1)t = \lambda_t(b_1 b_2)t$, implying that the proportionality constant satisfies the functional equation

$$\lambda_t(b_2)\lambda_t(b_1) = \lambda_t(b_1 b_2), \quad (2.217a)$$

$$\lambda_t(1) = 1, \quad (2.217b)$$

and similarly for the proportionality constant of the reduced external field.

The unique functional solution to this equation is a power law, see Appendix C, so that

$$t' = b^{y_t} t \quad \text{for } t \rightarrow 0^\pm, \text{ with } y_t > 0, \quad (2.218a)$$

$$h' = b^{y_h} h \quad \text{for } h \rightarrow 0^\pm, \text{ with } y_h > 0. \quad (2.218b)$$

The exponents y_t and y_h are positive since the flow is directed away from the critical point. The exponent y_t describing the flow of the temperature away from the critical temperature is in fact related to the critical exponent ν . Upon renormalisation, the correlation length is reduced by a factor b ,

$$\xi' = \frac{\xi}{b}. \quad (2.219)$$

The correlation length $\xi(t, 0) = \text{constant } |t|^{-\nu}$ as $t \rightarrow 0^\pm$, so that

$$\text{constant } |t'|^{-\nu} = \frac{\text{constant } |t|^{-\nu}}{b} \quad \text{for } t \rightarrow 0^\pm, h = 0. \quad (2.220)$$

Substituting $t' = b^{y_t} t$ and rearranging, we find $b^{1-\nu y_t} = 1$. Since $b > 1$ is arbitrary, the exponent must be zero and we conclude that

$$y_t = \frac{1}{\nu}. \quad (2.221)$$

Real space RG: free energy

With respect to the partition function, the coarse graining amounts to summing over all those configurations $\{s_i\}$ in the original lattice which are consistent with a particular block spin configuration $\{s_I\}$ in the renormalised lattice. The calculation of the partition function is then completed by summing over all possible block spin configurations,

$$\begin{aligned} Z(t, h, N) &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\ &= \sum_{\{s_I\}} \sum_{\substack{\text{configurations } \{s_i\} \\ \text{consistent with } \{s_I\}}} \exp(-\beta E_{\{s_i\}}). \end{aligned} \quad (2.222)$$

Defining the energy of the Ising model in the renormalised lattice, $E'_{\{s_I\}}$, through the equation

$$\exp(-\beta E'_{\{s_I\}}) = \sum_{\substack{\text{configurations } \{s_i\} \\ \text{consistent with } \{s_I\}}} \exp(-\beta E_{\{s_i\}}), \quad (2.224)$$

and substituting into Equation (2.222) we have that the partition function remains invariant under the real-space renormalisation transformation

$$\begin{aligned} Z(t, h, N) &= \sum_{\{s_I\}} \exp(-\beta E'_{\{s_I\}}) \\ &= Z(t', h', N'). \end{aligned} \quad (2.225)$$

Since the partition function remains invariant under renormalisation, so does the total free energy. However, the free energy per spin renormalises according to

$$\begin{aligned} f(t, h) &= -\frac{1}{N} k_B T \ln Z(t, h, N) \\ &= -b^{-d} \frac{1}{N'} k_B T \ln Z(t', h', N') \\ &= b^{-d} f(t', h'). \end{aligned} \quad (2.226)$$

Substituting Equations (2.218) into Equation (2.226) gives

$$f(t, h) = b^{-d} f(b^{y_t} t, b^{y_h} h) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0. \quad (2.227)$$

The singular part of the free energy per spin transforms as a generalised homogeneous function in the vicinity of the critical point. Although the free energy per spin consists of regular and singular parts, it is the latter that is responsible for the critical behaviour. For the purposes of obtaining the Widom scaling ansatz in Equation (2.168), we concentrate on the singular part of the free energy per spin which, from Equation (2.227), obeys

$$f_s(t, h) = b^{-d} f_s(b^{y_t} t, b^{y_h} h) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0. \quad (2.228)$$

Equation (2.228) implies the Widom scaling ansatz. The right-hand side is a function of two variables but can be recast as a function of one variable by setting the block size $b = |t|^{-1/y_t} \propto \xi$ in Equation (2.228),

$$\begin{aligned} f_s(t, h) &= \left[|t|^{-1/y_t} \right]^{-d} f_s \left(\left[|t|^{-1/y_t} \right]^{y_t} t, \left[|t|^{-1/y_t} \right]^{y_h} h \right) \\ &= |t|^{\nu d} f_s \left(t/|t|, h/|t|^{y_h/y_t} \right) \\ &= |t|^{\nu d} f_s \left(\pm 1, h/|t|^{y_h/y_t} \right) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0. \end{aligned} \quad (2.229)$$

Summary

By comparing with Equation (2.168) we make the identifications

$$2 - \alpha = \nu d, \quad (2.230a)$$

$$\Delta = y_h/y_t, \quad (2.230b)$$

$$\mathcal{F}_\pm(h/|t|^\Delta) = f_s(\pm 1, h/|t|^{y_h/y_t}), \quad (2.230c)$$

so that we recover the Widom scaling ansatz

$$f_s(t, h) = |t|^{2-\alpha} \mathcal{F}_\pm(h/|t|^\Delta) \quad \text{for } t \rightarrow 0^\pm, h \rightarrow 0. \quad (2.231)$$

The two branches of the scaling function for the free energy per spin for $t \rightarrow 0^\pm$ appear naturally as a result of the first argument in the free energy per spin on the right-hand side of Equation (2.230c).

In summary, the renormalised partition function takes the same form as the original partition function but with rescaled parameters. This implies that the free energy per spin is a generalised homogeneous function. Together with Equations (2.218), this provides an explanation for the Widom scaling ansatz in Equation (2.168) and the hyperscaling relation.

Renormalization: Ising chain d=1 & b=2

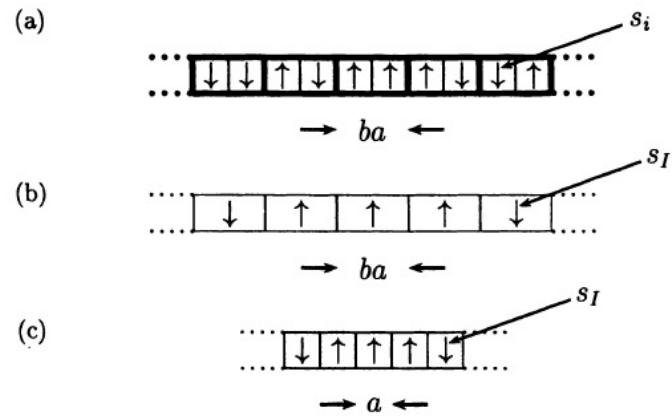
Consider the $d = 1$ Ising model of N spins with periodic boundary conditions in zero external field [Nelson and Fisher, 1975]. The partition function

$$\begin{aligned} Z(K_1, N) &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\ &= \sum_{\{s_i\}} \exp \left(K_1 \sum_{i=1}^N s_i s_{i+1} \right), \end{aligned} \quad (2.240)$$

where the reduced nearest-neighbour coupling constant,⁹ K_1 , is given by

$$K_1 = \beta J = \frac{J}{k_B T}. \quad (2.241)$$

First, we divide the lattice into blocks of size $b = 2$ each containing two spins, see Figure 2.33(a). Second, we replace each block of spins with a single block spin s_I which takes the value of the odd spin, see Figure 2.33(b). This choice is arbitrary and constitutes a decimation coarsening rule. Third, all length scales are reduced by the factor $b = 2$ to restore the original lattice spacing. We are left with a renormalised system with $N' = N/2$ spins where $\{s_I\}$ are the odd spins in the original lattice, see Figure 2.33(c).



Renormalization: Ising chain

To determine the partition function for the renormalised system, we sum out (integrate over) even spins in the original lattice so that only the odd spins in each block survives. Since each spin has two nearest neighbours, each spin appears twice in the exponent. Collecting each even spin in a single term, we find

$$\begin{aligned} Z(K_1, N) &= \sum_{\text{odd spins}} \sum_{\text{even spins}} \exp \left(K_1 \sum_{i=1}^N s_i s_{i+1} \right) \\ &= \sum_{\text{odd spins}} \sum_{\text{even spins}} \exp (K_1[s_1 s_2 + s_2 s_3]) \cdots \exp (K_1[s_{N-1} s_N + s_N s_1]) \\ &= \sum_{\text{odd spins}} 2 \cosh (K_1[s_1 + s_3]) \cdots 2 \cosh (K_1[s_{N-1} + s_1]), \quad (2.242) \end{aligned}$$

where the coarse graining sum over each of the even spins is readily performed. For example, for the spin s_2 that couples to spins s_1 and s_3 ,

$$\sum_{s_2=\pm 1} \exp (K_1 s_2 [s_1 + s_3]) = 2 \cosh (K_1 [s_1 + s_3]). \quad (2.243)$$

The pair of spins (s_1, s_3) can be in one of $2^2 = 4$ microstates. However, the right-hand side of this equation takes only two different values because of symmetry, and may be written with two appropriately defined renormalised (reduced) coupling constants K'_0 and K'_1 in the form

$$2 \cosh (K_1 [s_1 + s_3]) = \exp (K'_0 + K'_1 s_1 s_3). \quad (2.244)$$

The two simultaneous equations that determine the renormalised coupling constants are

$$2 \cosh 2K_1 = \exp (K'_0 + K'_1) \quad \text{for } s_1 = s_3, \quad (2.245a)$$

$$2 = \exp (K'_0 - K'_1) \quad \text{for } s_1 = -s_3. \quad (2.245b)$$

Solving for K'_0 and K'_1 in terms of K_1 , we find

$$K'_0 = \ln \left(2 \sqrt{\cosh 2K_1} \right), \quad (2.246a)$$

$$K'_1 = \frac{1}{2} \ln(\cosh 2K_1). \quad (2.246b)$$

Renormalization: Ising chain

Therefore, expressing the partition function in terms of the renormalised coupling constants

$$\begin{aligned} Z(K_1, N) &= \sum_{\text{odd spins}} \exp(K'_0 + K'_1 s_1 s_3) \cdots \exp(K'_0 + K'_1 s_{N-1} s_1) \\ &= \exp(N' K'_0) \sum_{\{s_I\}} \exp\left(K'_1 \sum_{I=1}^{N'} s_I s_{I+1}\right) \\ &= \exp(N' K'_0) Z(K'_1, N'). \end{aligned} \quad (2.247)$$

In the penultimate line, the odd spins s_1, s_3, \dots, s_{N-1} in the original lattice are relabelled as s_I in the renormalised lattice, with $I = 1, \dots, N'$. Factorising out the constant $\exp(N' K'_0)$, we recognise that the summation term takes the same form as the partition function for the original system but with a reduced number of spins $N' = N/b$ and a renormalised coupling constant $K'_1 < K_1$ given by Equation (2.246b).

The entire expression in the last line of Equation (2.247) is the partition function for the renormalised system. The total free energy remains the same after renormalisation and, in units of $k_B T$, is given by

$$-\ln Z(K_1, N) = -N' K'_0 - \ln Z(K'_1, N'), \quad (2.248)$$

where the term $N' K'_0$ appears explicitly as a free energy offset. However, when calculating probabilities and ensemble averages, the constant $\exp(N' K'_0)$ cancels out and plays no role.

How does the renormalised system behave compared to the original system? The renormalisation of the coupling constant in Equation (2.246b) implies that

$$K'_1 < K_1 \quad \text{for } K_1 > 0. \quad (2.249)$$

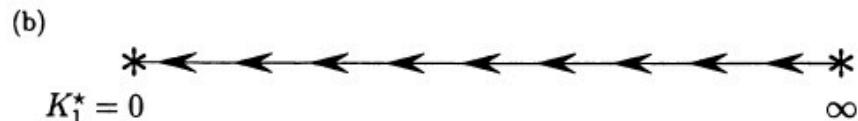
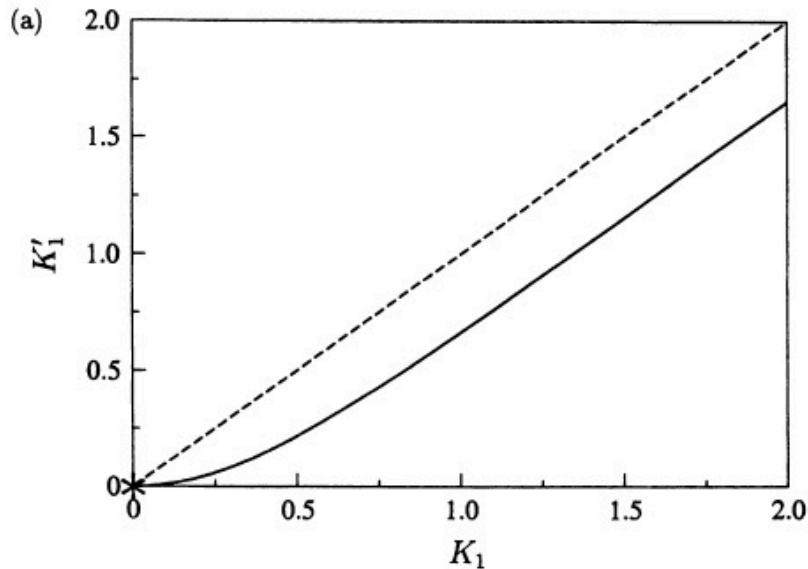
This manifests itself in Figure 2.34(a) in that the graph of the renormalised coupling constant K'_1 lies below the dashed line $K'_1 = K_1$ for all $K_1 > 0$. Therefore, the coupling between nearest-neighbour spins in the renormalised lattice is weaker than between nearest-neighbour spins in the original lattice. The renormalisation procedure can be readily applied again and again with the effect that the coupling constant becomes weaker and weaker.

Successive applications of the renormalisation procedure induces a flow in the coupling constant towards the fixed point $K_1^* = 0$, see Figure 2.34(b).

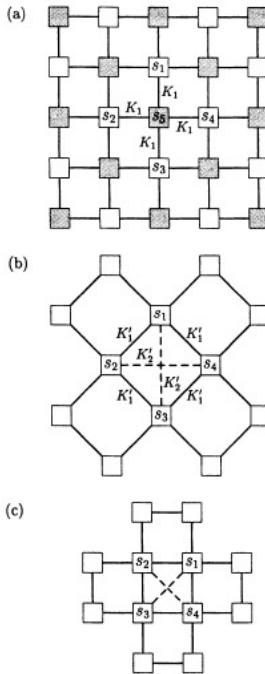
RG flow

(a) The renormalised coupling constant, K' , in the one-dimensional Ising model in zero external field versus the coupling constant in the original lattice, K . The fixed points (K^*) lie at the intersections between the graph for K' and the dashed line $K' = K$. The fixed point $K^* = \infty$ is not visible.

(b) The associated renormalisation group transformation flow in K -space. In the renormalised lattice, nearest-neighbour spins couple with strength $K' < K$. The fixed point $K^* = \infty$ is unstable. For $0 < K < \infty$, applying the renormalisation group transformation will induce a flow towards the stable fixed point $K^* = 0$.



Renormalization: Ising on a square lattice ($b=2$)



Consider the $d = 2$ Ising model of N spins on a square lattice in zero external field [Maris and Kadanoff, 1978]. The partition function

$$\begin{aligned} Z(K_1, N) &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\ &= \sum_{\{s_i\}} \exp \left(K_1 \sum_{\langle ij \rangle} s_i s_j \right), \end{aligned} \quad (2.250)$$

where $K_1 = J/(k_B T)$ is the reduced nearest-neighbour coupling constant and the sum in the exponential runs over all distinct nearest-neighbour pairs.

We apply a renormalisation transformation where the coarse graining is effected by summing out every second spin in the original lattice, which is a realisation of a decimation coarsening rule. In Figure 2.35(a), the decimated spins, that is, the spins to be summed over, have been shaded dark grey. Note that each pair of remaining spins, for example (s_1, s_2) , has two common nearest neighbours of decimated spins. The remaining spins form a square lattice rotated by 45° with lattice constant $ba = \sqrt{2}a$, see Figure 2.35(b). To complete the renormalisation transformation, all length scales are reduced by the factor $b = \sqrt{2}$ to restore the original lattice spacing. After a 45° clockwise rotation, we are left with a renormalised version of the original system with $N' = N/b^2$ spins, see Figure 2.35(c).

Renormalization: Ising square lattice

To determine the partition function for the renormalised system, we have to perform the coarse graining explicitly by summing over every second spin. Since each spin has four nearest neighbours, each spin appears four times in the exponent of the exponential.

Collecting each decimated spin in a single term, we find

$$\begin{aligned} Z(K_1, N) &= \sum_{\text{remaining spins}} \sum_{\text{decimated spins}} \exp \left(K_1 \sum_{\langle ij \rangle} s_i s_j \right) \\ &= \sum_{\text{remaining spins}} \sum_{\text{decimated spins}} \cdots \exp (K_1 s_5 [s_1 + s_2 + s_3 + s_4]) \cdots \\ &= \sum_{\text{remaining spins}} \cdots 2 \cosh (K_1 [s_1 + s_2 + s_3 + s_4]) \cdots, \end{aligned} \quad (2.251)$$

where the coarse graining over each decimated spins is readily performed. For example, for the spin s_5 that couples to spins s_1, s_2, s_3, s_4 , see Figure 2.35(a), we find

$$\sum_{s_5=\pm 1} \exp (K_1 s_5 [s_1 + s_2 + s_3 + s_4]) = 2 \cosh (K_1 [s_1 + s_2 + s_3 + s_4]). \quad (2.252)$$

The quadruple of spins (s_1, s_2, s_3, s_4) can be in one of $2^4 = 16$ microstates. However, the right-hand side of this equation takes only three different values because of symmetry, and may be written with four appropriately defined renormalised coupling constants K'_0, K'_1, K'_2 and K'_3 in the form

$$\begin{aligned} 2 \cosh (K_1 [s_1 + s_2 + s_3 + s_4]) &= \\ \exp \left(K'_0 + \frac{K'_1}{2} [s_1 s_2 + s_1 s_4 + s_2 s_3 + s_3 s_4] + K'_2 [s_1 s_3 + s_2 s_4] + K'_3 s_1 s_2 s_3 s_4 \right). \end{aligned} \quad (2.253)$$

Just as in the one-dimensional case, the coarse graining generates a constant coupling term K'_0 which only plays a role as a free energy offset that does not affect the calculation of probabilities and ensemble averages. Similarly, the nearest-neighbour coupling constant K_1 is renormalised to become K'_1 .

This is not all, however. Contrary to one dimension, the coarse graining in two dimensions generates, in addition, renormalised coupling constants K'_2 , representing next-nearest-neighbour (nnn) interactions and K'_3 , representing quadruple (\square) interactions.

Renormalization: Ising square lattice

Physically, the introduction of these extra coupling constants K'_2 and K'_3 can be understood with reference to Figure 2.35(a). For example, spins s_1 and s_3 interact indirectly through spin s_5 . Therefore, when summing out spin s_5 , an effective coupling K'_2 between s_1 and s_3 must be introduced. Likewise, the quadruple of spins s_1, s_2, s_3, s_4 interact indirectly through spin s_5 . Therefore, when summing out spin s_5 , an effective coupling K'_3 between s_1, s_2, s_3, s_4 must also be introduced.

The four simultaneous equations that determine the renormalised coupling constants are

$$\begin{aligned} 2 \cosh 4K_1 &= \exp(K'_0 + 2K'_1 + 2K'_2 + K'_3) & \left\{ \begin{array}{l} s_1 = s_2 = s_3 = s_4, \\ -s_1 = s_2 = s_3 = s_4, \\ s_1 = -s_2 = s_3 = s_4, \\ s_1 = s_2 = -s_3 = s_4, \\ s_1 = s_2 = s_3 = -s_4, \end{array} \right. \\ 2 \cosh 2K_1 &= \exp(K'_0 - K'_3) & \left\{ \begin{array}{l} s_1 = -s_2 = -s_3 = s_4, \\ s_1 = s_2 = -s_3 = -s_4, \end{array} \right. \\ 2 &= \exp(K'_0 - 2K'_2 + K'_3) & \left\{ \begin{array}{l} s_1 = -s_2 = -s_3 = s_4, \\ s_1 = s_2 = -s_3 = -s_4, \end{array} \right. \\ 2 &= \exp(K'_0 - 2K'_1 + 2K'_2 + K'_3) & \left\{ \begin{array}{l} s_1 = -s_2 = s_3 = -s_4. \end{array} \right. \end{aligned}$$

Each of the eight conditions specifies two microstates of the quadruple of spins. For example, $-s_1 = s_2 = s_3 = s_4$ specifies either $(-1, +1, +1, +1)$ or $(+1, -1, -1, -1)$.

Solving for K'_0, K'_1, K'_2 and K'_3 in terms of K_1 , we find after some algebra

$$K'_0 = \ln \left(2\sqrt{\cosh 2K_1} (\cosh 4K_1)^{1/8} \right), \quad (2.254a)$$

$$K'_1 = \frac{1}{4} \ln (\cosh 4K_1), \quad (2.254b)$$

$$K'_2 = \frac{1}{8} \ln (\cosh 4K_1), \quad (2.254c)$$

$$K'_3 = \frac{1}{8} \ln (\cosh 4K_1) - \frac{1}{2} \ln (\cosh 2K_1). \quad (2.254d)$$

Therefore, the partition function can be expressed in terms of the renormalised coupling constants.

Note that an additional term of $\exp(K'_1/2[s_1s_2 + s_1s_4 + s_2s_3 + s_3s_4])$ arises from the additional common nearest neighbour for each pair of the remaining spin $(s_1, s_2), (s_1s_4), (s_2, s_3), (s_3, s_4)$, see Figure 2.35(a).

Renormalization: Ising square lattice

Relabelling the remaining spins from the original lattice as s_I, s_J, \dots and factoring out the constant $\exp(N'K'_0)$, we have

$$\begin{aligned} Z(K_1, N) &= \exp(N'K'_0) \sum_{\{s_I\}} \exp \left(K'_1 \sum_{\langle IJ \rangle} s_I s_J + K'_2 \sum_{\text{nnn}} s_I s_J + K'_3 \sum_{\square} s_I s_J s_K s_L \right) \\ &= \exp(N'K'_0) Z(K'_1, K'_2, K'_3, N'), \end{aligned} \quad (2.255)$$

where the sums in the exponential run over all distinct nearest-neighbour and next-nearest-neighbour pairs and quadruples, respectively. Without the couplings K'_2, K'_3 , the sum over block spin configurations $\{s_I\}$ takes the same functional form as the original partition function but with a reduced number of spins $N' = N/b^2$ and a renormalised coupling constant K'_1 given by Equation (2.254b). With the couplings K'_2, K'_3 , however, the energy $E_{\{s_I\}}$ must be generalised to include next-nearest-neighbour and quadruple spin interactions for the sum over block spin configurations $\{s_I\}$ to be identified with a partition function $Z(K'_1, K'_2, K'_3, N')$, see Equation (2.250).

In fact, upon successive applications of the renormalisation transformation, the coupling constants K'_0, K'_1, K'_2 and K'_3 are renormalised in turn and additional renormalised coupling constants are generated at each iteration. As a result, the energy must be generalised still further to include all possible spin interactions of which there are, in principle, infinitely many.

The possible spin interactions must respect the symmetry of the problem. In the Ising model in zero external field, for example, the energy must be invariant under the reversal of spins $s_i \mapsto -s_i$, thereby precluding interaction terms with an odd number of spins, such as $s_i s_j s_k$. In Section 2.16 we present a general theory of real-space renormalisation group transformations that will allow for an infinite number of couplings.

In order to calculate the partition function for the two-dimensional Ising model exactly, all generated couplings must be retained. However, let us investigate whether a truncated coupling space can yield a phase transition at non-zero temperature.

The most drastic approximation is to ignore all the generated couplings. After setting $K'_2 = K'_3 = \dots = 0$, the flow of the remaining coupling constants is described by

$$K'_0 = \ln \left(2\sqrt{\cosh 2K_1} (\cosh 4K_1)^{1/8} \right), \quad (2.256a)$$

$$K'_1 = \frac{1}{4} \ln (\cosh 4K_1). \quad (2.256b)$$

Renormalization: Ising square lattice

Equation (2.256b) is similar to Equation (2.246b) describing the flow in the one-dimensional case and has only two fixed points: an unstable low-temperature fixed point $K_1^* = \infty$ and a stable high-temperature fixed point $K_1^* = 0$. Only the low- and high-temperature fixed points survive this crude truncation of the coupling space. Therefore, when ignoring all the generated couplings, the renormalisation transformation incorrectly predicts that there is no phase transition in zero external field for any finite temperature in the $d = 2$ Ising model.

A less drastic approximation is to ignore all the generated couplings, except K'_2 . After setting $K'_3 = \dots = 0$, the flow of the remaining coupling constants is described by

$$K'_0 = \ln \left(2\sqrt{\cosh 2K_1} (\cosh 4K_1)^{1/8} \right), \quad (2.257a)$$

$$K'_1 = \frac{1}{4} \ln (\cosh 4K_1), \quad (2.257b)$$

$$K'_2 = \frac{1}{8} \ln (\cosh 4K_1). \quad (2.257c)$$

Both coupling constants K'_1 and K'_2 are positive and favour the alignment of spins. It is therefore reasonable to combine their effect into a single coupling constant \tilde{K}'_1 . To estimate how much of a contribution K'_2 makes in the effective nearest-neighbour coupling constant \tilde{K}'_1 , consider a system of fully aligned spins. Since there are $N'z/2$ different nearest-neighbour and next-nearest-neighbour pairs, the renormalised reduced energy (without the constant offset $N'K'_0$)

$$\begin{aligned} E_{\{s_I\}} &= K'_1 \sum_{(IJ)} s_I s_J + K'_2 \sum_{nnn} s_I s_J \\ &= (K'_1 + K'_2) \frac{N'z}{2}. \end{aligned} \quad (2.258)$$

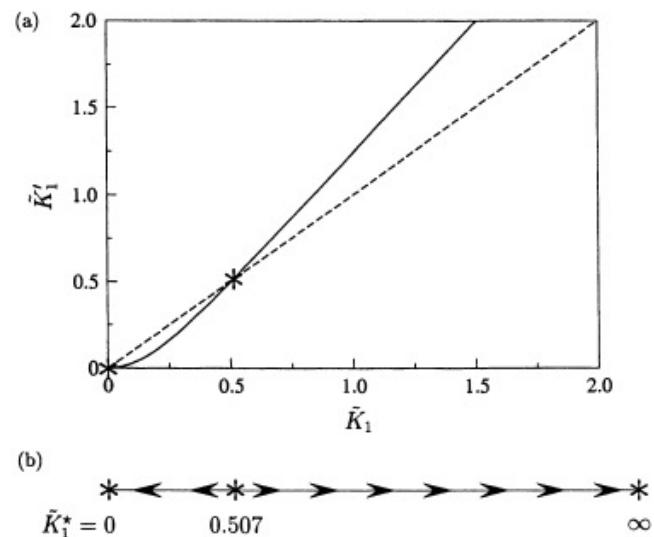
Therefore, the effective nearest-neighbour coupling constant

$$\begin{aligned} \tilde{K}'_1 &= K'_1 + K'_2 \\ &= \frac{3}{8} \ln \left(\cosh 4\tilde{K}_1 \right). \end{aligned} \quad (2.259)$$

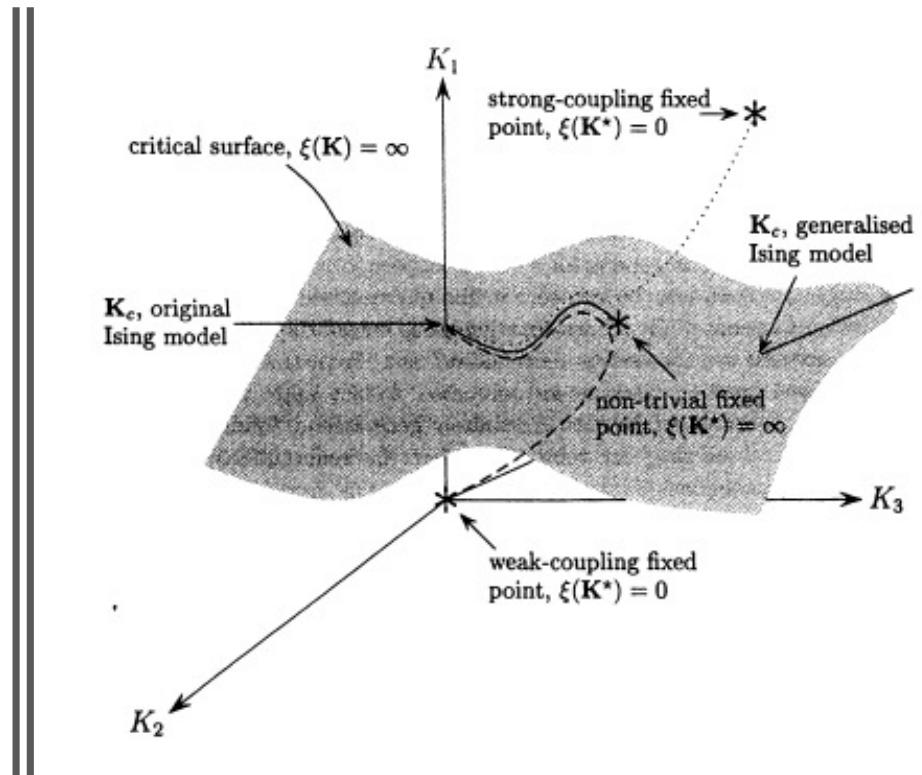
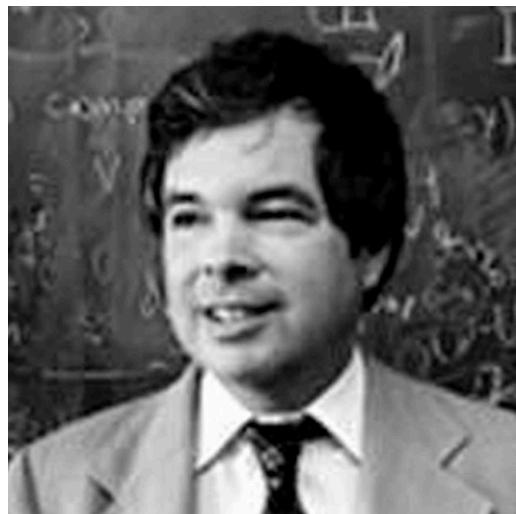
RG flow

(a) The renormalised coupling constant, K' , for the two-dimensional Ising model on a square lattice in zero external field versus the coupling constant in the original lattice, K . The fixed points (*) lie at the intersections between the graph for K' and the dashed line $K' = K$. The fixed point $K^* = \infty$ is not visible.

(b) The associated renormalisation transformation flow in K -space. The fixed point $K^* = 0.507$ is unstable. For $0 < K < 0.507$, applying the renormalisation transformation will induce a flow towards the stable fixed point $K^* = 0$. For $K > 0.507$, applying the renormalisation transformation will induce a flow towards the stable fixed point $K^* = \infty$.



Wilson's renormalization group theory



Wilson's RG theory

Similarly, applying the renormalisation group transformation once to the two-dimensional Ising model reduces the degrees of freedom from N to $N' = N/b^2$, and generates a renormalised nearest-neighbour coupling constant K'_1 and a constant coupling term K'_0 . However, in contrast to one dimension, next-nearest neighbour interactions K'_2 and quadruple spin interactions K'_3 are generated in addition – even though $K_2 = K_3 = 0$ in the original system. In general for $d > 1$, a coupling constant that is zero in the original system may be non-zero in the renormalised system. On successive applications of the renormalisation group transformation, these coupling constants are themselves renormalised and, furthermore, additional renormalised coupling constants are generated. In fact, applying the renormalisation group transformation indefinitely generates an infinite number of renormalised coupling constants. Therefore, the renormalisation group transformation applied to the two-dimensional Ising model is associated with a flow in an infinite-dimensional coupling space:

$$\begin{aligned} K_1 &\mapsto K'_1 \mapsto K_1^{(2)} \mapsto \cdots \mapsto K_1^{(n-1)} \mapsto K_1^{(n)} \mapsto \cdots \\ 0 = K_2 &\mapsto K'_2 \mapsto K_2^{(2)} \mapsto \cdots \mapsto K_2^{(n-1)} \mapsto K_2^{(n)} \mapsto \cdots \quad (2.261) \\ 0 = K_3 &\mapsto K'_3 \mapsto K_3^{(2)} \mapsto \cdots \mapsto K_3^{(n-1)} \mapsto K_3^{(n)} \mapsto \cdots \\ &\vdots \end{aligned}$$

This motivates the introduction of an infinite-dimensional coupling space consisting of all possible coupling constants

$$\mathbf{K} = (K_1, K_2, K_3, \dots), \quad (2.262)$$

see Figure 2.37. Since the constant coupling term is not on the same footing as all the other coupling constants, it is not included in the coupling space. Physically, the constant coupling term represents a contribution to the free energy arising from summing out the degrees of freedom over the short length scale ba . Even though the constant coupling term neither affects expectation values nor is included in the coupling space, it plays a vital role of its own since its contribution to the free energy guarantees that the formalism is self-consistent.

For the following discussion, recall that the coupling constants are proportional to $1/(k_B T)$. Consider the ‘original’ Ising model at a given temperature T in zero external field with coupling constant $\mathbf{K} = (K_1, 0, 0, \dots)$ represented by a point lying on the K_1 -axis in the infinite-dimensional coupling space, see Figure 2.37. The temperature determines where the

Wilson's RG theory

Now, consider a ‘generalised’ Ising model at a given temperature T in zero external field with coupling constant $\mathbf{K} = (K_1, K_2, K_3, \dots)$ represented by a point in the infinite-dimensional coupling space. The temperature determines where the particular generalised Ising model lies along the line from the origin in the direction given by \mathbf{K} , see Figure 2.37. If $T = \infty$, the coupling constant $\mathbf{K} = (0, 0, 0, \dots)$ and the associated correlation length $\xi(\mathbf{K}) = 0$. Therefore, the weak-coupling (high-temperature) generalised Ising model lies at the origin. If $T = T_c$, the coupling constant takes its critical value $\mathbf{K}_c = (K_{1c}, K_{2c}, K_{3c}, \dots)$ and the associated correlation length $\xi(\mathbf{K}_c) = \infty$. If $T = 0$, the coupling constant $\mathbf{K} = (\infty, \infty, \infty, \dots)$ and the associated correlation length $\xi(\mathbf{K}) = 0$. The strong-coupling (low temperature) generalised Ising model lies at infinity.

Now that we have become familiar with the infinite-dimensional coupling space, we can show that the repeated application of the renormalisation group transformation on a generalised Ising model can be visualised as a discrete flow in this space.

As a starting point, consider a generalised Ising model in zero external field that allows for an infinite number of coupling constants representing nearest-neighbour interactions, next-nearest-neighbour interactions, quadruple spins interactions, etc. Such a generalised Ising model is defined by a coupling constant \mathbf{K} and a constant coupling term K_0 . The associated generalised reduced energy takes the form¹¹

$$-\beta E_{\{s_i\}} = K_0 N + K_1 \sum_{(ij)} s_i s_j + K_2 \sum_{\text{nnn}} s_i s_j + K_3 \sum_{\square} s_i s_j s_k s_l + \dots \quad (2.263)$$

The generalised reduced energy contains all possible spin interactions, of which there are infinitely many, respecting the symmetry of the problem: in zero external field, for example, interaction terms with an odd number of spins, such as $s_i s_j s_k$, cannot be present since the energy must be invariant under the reversal of spins $s_i \mapsto -s_i$; however, all interaction terms with an even number of spins, such as $s_i s_j s_k s_l$, are present. Note that we may

Wilson's RG theory

Applying the renormalisation group transformation once to a generalised Ising model renormalises the associated reduced energy. The reduced energy in the renormalised system, $\beta E'_{\{s_I\}}$, is defined through the equation

$$\begin{aligned} -\beta E'_{\{s_I\}} &= \ln \left[\sum_{\substack{\text{configurations } \{s_I\} \\ \text{consistent with } \{s_I\}}} \exp(-\beta E_{\{s_I\}}) \right] \quad (2.264) \\ &= K'_0 N' + K'_1 \sum_{(IJ)} s_I s_J + K'_2 \sum_{\text{nnn}} s_I s_J + K'_3 \sum_{\square} s_I s_J s_K s_L + \dots \end{aligned}$$

The renormalisation group transformation reduces the degrees of freedom from N to $N' = N/b^d$ block spin variables $\{S_I\}$, whose couplings are given by the renormalised coupling constants $\mathbf{K}' = (K'_1, K'_2, K'_3, \dots)$ and, in addition, the spin-independent term renormalises to $K'_0 N'$. Note that, in contrast to the Kadanoff block spin transformation, this general formulation allows for ‘new’ coupling constants to be generated.

Let us now formally introduce the renormalisation group transformation R_b as a transformation acting on the members of the infinite-dimensional coupling space, that effects coarse-graining over blocks of size ba :

$$\mathbf{K}' = R_b(\mathbf{K}). \quad (2.265)$$

Equation (2.265) expresses a recursion relation that can be applied indefinitely on a system in the thermodynamic limit. Since the renormalisation group transformation involves a coarse-graining procedure over a block with a finite number of b^d spins, the transformation is analytic. This analyticity will allow for a Taylor expansion of R_b which will prove important shortly. However, if the renormalisation group transformation is applied indefinitely to a system in the thermodynamic limit, singular behaviour may occur. In this respect the renormalisation group transformation is able to account for critical phenomena. Note also that renormalising twice, first with R_b , and then with R_{b_2} , is equivalent to renormalising once with $R_{b_1 b_2}$. The renormalisation group transformation therefore satisfies $R_{b_2}(R_{b_1}(\mathbf{K})) = R_{b_1 b_2}(\mathbf{K})$ for all \mathbf{K} . Expressed as an operator identity:¹²

$$R_{b_2} R_{b_1} = R_{b_1 b_2}. \quad (2.266)$$

Self-similarity & fixed points

A fixed point of the renormalisation group transformation is a point \mathbf{K}^* in the infinite-dimensional coupling space that is invariant under renormalisation, that is,

$$R_b(\mathbf{K}^*) = \mathbf{K}^*. \quad (2.268)$$

Equation (2.268) is the fixed point equation for the renormalisation group transformation. For a fixed point \mathbf{K}^* , the associated reduced energy is invariant under renormalisations; hence, the associated generalised Ising model is invariant under rescaling. We will show that the fixed points of the renormalisation group transformation are associated with zero or infinite correlation length. Hence, as in percolation, self-similarity and scale invariance are associated with the fixed points of the renormalisation group transformation.

The discrete flow in the infinite-dimensional space of coupling constants generated by applying the renormalisation group transformation is associated with a flow in the correlation length. Applying the renormalisation group transformation once reduces the correlation length from $\xi(\mathbf{K})$ to $\xi(\mathbf{K}')$ where

$$\xi(\mathbf{K}') = \frac{\xi(\mathbf{K})}{b}. \quad (2.269)$$

Since the correlation length after each application of the renormalisation group transformation is reduced by the rescaling factor b , after n successive transformations

$$\xi[R_b^n(\mathbf{K})] = \frac{\xi(\mathbf{K})}{b^n}, \quad \text{for } n = 1, 2, \dots \quad (2.270)$$

If the initial correlation length is finite, $\xi(\mathbf{K}) < \infty$, then the correlation length after n transformations is reduced by a factor b^n and the renor-

Self-similarity & fixed points

malised system moves further and further away from criticality, disclosing the large scale behaviour of the original system. The correlation length eventually shrinks to zero as $n \rightarrow \infty$. If, however, the initial correlation length is infinite, $\xi(\mathbf{K}) = \infty$, then so too is the correlation length in all the renormalised systems.

We will now show that a system with no characteristic scale is a fixed point of the renormalisation group transformation and vice versa.

Applying the renormalisation group transformation indefinitely,

$$\xi \left[\lim_{n \rightarrow \infty} R_b^n(\mathbf{K}) \right] = \lim_{n \rightarrow \infty} \frac{\xi(\mathbf{K})}{b^n} = \begin{cases} 0 & \text{for } \xi(\mathbf{K}) < \infty \\ \infty & \text{for } \xi(\mathbf{K}) = \infty. \end{cases} \quad (2.271)$$

The correlation length associated with the generalised Ising model corresponding to the point $\lim_{n \rightarrow \infty} R_b^n(\mathbf{K})$ in coupling space is zero or infinite so there is no characteristic scale associated with $\lim_{n \rightarrow \infty} R_b^n(\mathbf{K})$. Therefore, $\lim_{n \rightarrow \infty} R_b^n(\mathbf{K})$ must be invariant under the renormalisation group transformation, that is,

$$R_b \left[\lim_{n \rightarrow \infty} R_b^n(\mathbf{K}) \right] = \lim_{n \rightarrow \infty} R_b^n(\mathbf{K}). \quad (2.272)$$

Equation (2.272) demonstrates that $\lim_{n \rightarrow \infty} R_b^n(\mathbf{K})$ satisfies the fixed point equation for the renormalisation group transformation and we identify

$$\mathbf{K}^* = \lim_{n \rightarrow \infty} R_b^n(\mathbf{K}), \quad (2.273)$$

with an associated correlation length that is $\xi(\mathbf{K}^*) = 0$ or $\xi(\mathbf{K}^*) = \infty$.

Now, assume that there exists a fixed point \mathbf{K}^* for the renormalisation group transformation. From Equation (2.269) we have $\xi(R_b(\mathbf{K}^*)) = \xi(\mathbf{K}^*)/b$, and after applying Equation (2.268) we find for the correlation length at a fixed point

$$\xi(\mathbf{K}^*) = \frac{\xi(\mathbf{K}^*)}{b} \Leftrightarrow \xi(\mathbf{K}^*) = \begin{cases} 0 & \text{'trivial'} \\ \infty & \text{'non-trivial'}. \end{cases} \quad (2.274)$$

In summary, a fixed point of the renormalisation group transformation implies that there is no characteristic scale; scale invariance prevails. Likewise, if scale invariance prevails, it is associated with a fixed point of the renormalisation group transformation.

Basin of attraction

In general, a renormalisation group transformation may have several fixed points. For simplicity, consider a renormalisation group transformation which has only three fixed points in the infinite-dimensional coupling space: the weak-coupling (high-temperature) fixed point $\mathbf{K}^* = (0, 0, 0, \dots)$ lying at the origin with $\xi(\mathbf{K}^*) = 0$, the strong-coupling (low-temperature) fixed point $\mathbf{K}^* = (\infty, \infty, \infty, \dots)$ lying at infinity with $\xi(\mathbf{K}^*) = 0$, and a non-trivial fixed point \mathbf{K}^* with $\xi(\mathbf{K}^*) = \infty$, see Figure 2.37.

Each of the fixed points \mathbf{K}^* will have a so-called basin of attraction, consisting of all points in the coupling space that flow into the fixed point \mathbf{K}^* when the renormalisation group transformation is applied indefinitely.

The basin of attraction of the non-trivial fixed point \mathbf{K}^* with $\xi(\mathbf{K}^*) = \infty$ is known as the ‘critical surface’ or, more generally the ‘critical manifold’, since its dimensionality need not be restricted to 2. We can show that for \mathbf{K} to lie in the basin of attraction of the non-trivial fixed point, its associated correlation length must be infinite, $\xi(\mathbf{K}) = \infty$. A simple rearrangement of Equation (2.270) yields

$$\xi(\mathbf{K}) = b^n \xi[R_b^n(\mathbf{K})]. \quad (2.275)$$

The correlation length at an initial point \mathbf{K} in coupling space is a factor b^n larger than the correlation length associated with the point after n transformations. The left-hand side of Equation (2.275) is independent of n . Therefore, if \mathbf{K} lies in the basin of attraction of the non-trivial fixed point \mathbf{K}^* with $\xi(\mathbf{K}^*) = \infty$, then taking the limit of $n \rightarrow \infty$ we find

$$\xi(\mathbf{K}) = \lim_{n \rightarrow \infty} b^n \xi[R_b^n(\mathbf{K})] = \lim_{n \rightarrow \infty} b^n \xi(\mathbf{K}^*) = \infty. \quad (2.276)$$

Hence, for \mathbf{K} to lie in the basin of attraction of the non-trivial fixed point, the associated correlation length must be infinite, that is, $\xi(\mathbf{K}) = \infty$. Equivalently, we may also define the critical surface as the set of all coupling constants \mathbf{K} where $\xi(\mathbf{K}) = \infty$. In Figure 2.37, the surface that has been shaded dark grey is part of the infinite critical surface.

The critical surface divides the coupling space into the basin of attraction of the weak-coupling fixed point, lying at the origin, consisting of all points ‘below’ the critical surface, the basin of attraction of the strong-coupling fixed point, lying at infinity, consisting of all points ‘above’ the critical surface, and finally the basin of attraction of the non-trivial critical fixed point, lying on the critical surface, consisting of all points on the critical surface, see Figure 2.37.

RG flow

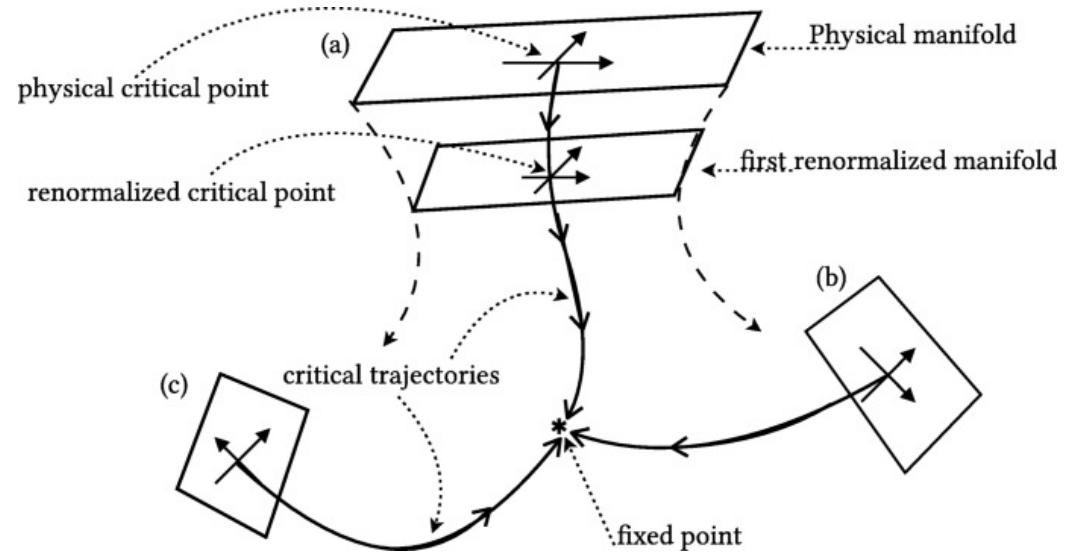
Consider the original Ising model in zero external field at reduced temperature t . If t is in the neighbourhood of the critical temperature $t = 0$, the model lies along the K_1 -axis in the neighbourhood of the critical surface in the infinite-dimensional coupling space, see Figure 2.37. Applying the renormalisation group transformation induces a discrete flow in coupling space. In Figure 2.32, we have seen the associated flow in configurational space for the two-dimensional Ising model with a particular choice of the renormalisation group transformation, namely the majority rule with $b = 3$.

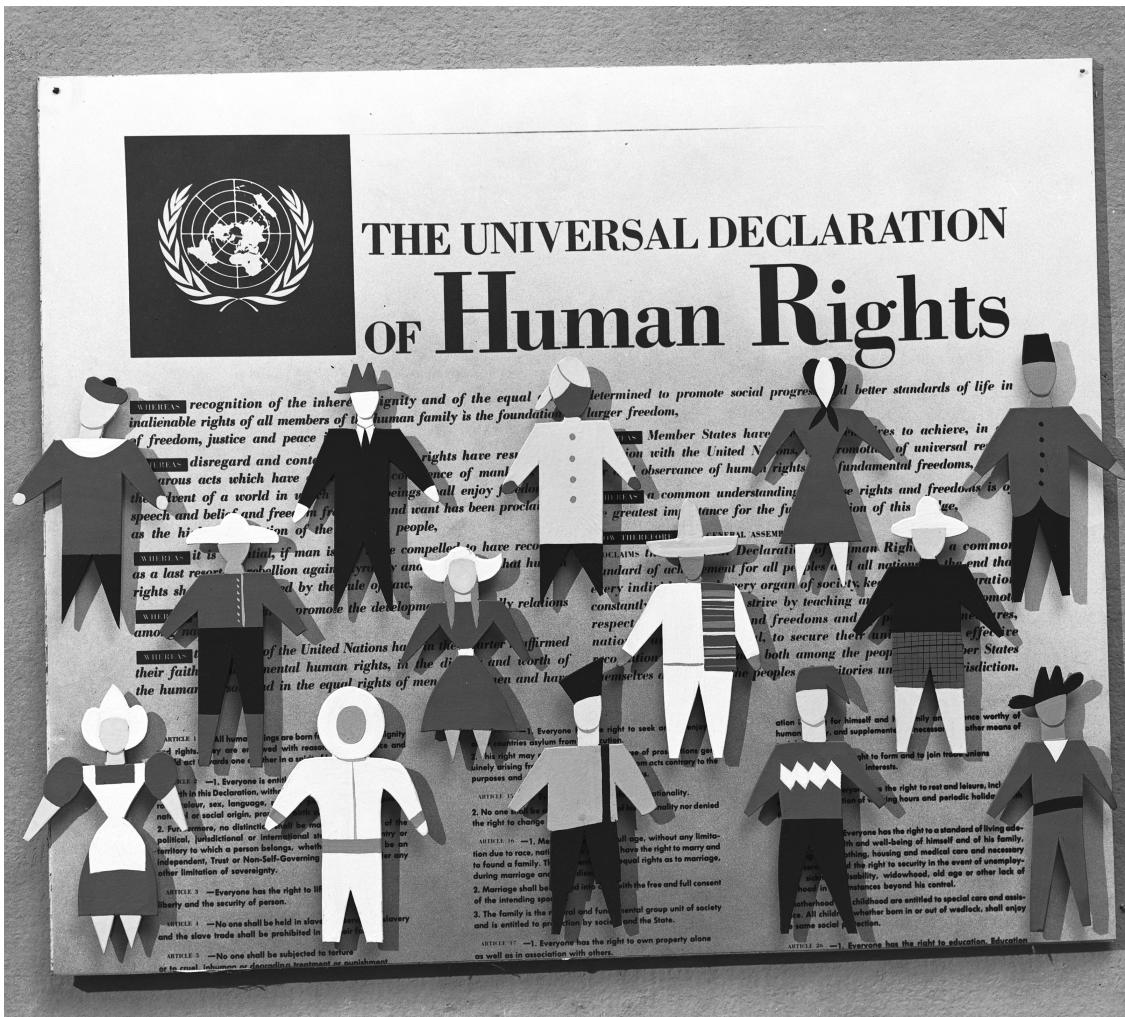
Assume that the initial temperature is slightly below the critical temperature, that is, $t < 0$. Applying the renormalisation group transformation repeatedly induces the flow in configurational space displayed in the left-hand column of Figure 2.32 towards the trivial fixed point of all spins aligned associated with $T = 0$. This flow in configurational space is associated with the discrete flow in coupling space along the dotted line commencing on the K_1 -axis just above the critical surface and ‘terminating’ at the strong-coupling fixed point $\mathbf{K}^* = (\infty, \infty, \infty, \dots)$ lying at infinity with correlation length $\xi(\mathbf{K}^*) = 0$. Therefore, the two microstates associated with $\mathbf{K}^* = (\infty, \infty, \infty, \dots)$ are trivially self-similar.

Next assume that the initial temperature is slightly above the critical temperature, that is, $t > 0$. Applying the renormalisation group transformation repeatedly induces the flow in configurational space displayed in the right-hand column of Figure 2.32 towards the trivial fixed point of randomly orientated spins associated with $T = \infty$. This flow in configurational space is associated with the discrete flow in coupling space along the dashed line commencing on the K_1 -axis just below the critical surface and terminating at the weak-coupling fixed point $\mathbf{K}^* = (0, 0, 0, \dots)$ lying at the origin with correlation length $\xi(\mathbf{K}^*) = 0$. Therefore, the microstates associated with $\mathbf{K}^* = (0, 0, 0, \dots)$ are trivially self-similar.

Finally, assume that the initial temperature is critical, that is, $t = 0$. Applying the renormalisation group transformation repeatedly does not induce a flow in configurational space, see the middle column of Figure 2.32. Nevertheless, the absence of flow in configurational space is associated with the flow in coupling space commencing on the K_1 -axis on the critical surface along the solid line terminating at the non-trivial fixed point \mathbf{K}^* with correlation length $\xi(\mathbf{K}^*) = \infty$. Therefore, the microstates associated with \mathbf{K}^* are self-similar.

RG flow





Universality

Universality

Assume that \mathbf{K}_c lies on the critical surface, that is, $\xi(\mathbf{K}_c) = \infty$. As we have just seen, it is not the initial critical value of the coupling constant nor the flow in the neighbourhood of \mathbf{K}_c that determines the critical behaviour of the associated generalised Ising model. Rather, the critical behaviour is determined by the flow of $R_b^n(\mathbf{K})$ for $n \rightarrow \infty$, which takes place in the neighbourhood of the non-trivial fixed point \mathbf{K}^* on the critical surface!

Each point \mathbf{K}_c on the critical surface represents a particular generalised Ising model at its critical point. However, since they all flow into the same non-trivial fixed point when applying the renormalisation group transformation indefinitely, their critical behaviour is determined by the flow close to this fixed point. Indeed, universality refers to the identical behaviour shown by systems close to the fixed point \mathbf{K}^* , rather than at the fixed point itself. Therefore, we need to investigate in more detail the flow in coupling space close to the non-trivial fixed point on the critical surface. In doing so, we will, as a by-product, also be able to demonstrate how the Widom scaling ansatz for the singular part of the free energy per spin can be derived using the general framework of the renormalisation group transformation.

Let $\mathbf{K} = \mathbf{K}^* + \delta\mathbf{K}$ be close to the fixed point \mathbf{K}^* , that is, the entries $\delta\mathbf{K}$ in the deviation from the fixed point are small. Applying the renormalisation group transformation once, $R_b(\mathbf{K}) = \mathbf{K}' = \mathbf{K}^* + \delta\mathbf{K}'$ where $\delta\mathbf{K}'$, the deviation from the fixed point after renormalisation, is a function of \mathbf{K} . Since \mathbf{K}^* is a fixed point of the renormalisation group transformation, we have

$$\begin{aligned} R_b(\mathbf{K}) &= \mathbf{K}^* + \delta\mathbf{K}' \\ &= R_b(\mathbf{K}^*) + \delta\mathbf{K}'. \end{aligned} \quad (2.277)$$

However, since R_b is analytic, we can Taylor expand the renormalisation group transformation around the fixed point \mathbf{K}^* , and to first order in $\delta\mathbf{K}$ we find

$$R_b(\mathbf{K}) = R_b(\mathbf{K}^*) + \mathbf{M}(b)\delta\mathbf{K} + \mathcal{O}(\delta\mathbf{K}^2), \quad (2.278)$$

where the ij th entry in the matrix $\mathbf{M}(b) = \partial\mathbf{K}'/\partial\mathbf{K}$

$$[\mathbf{M}(b)]_{ij} = \left. \frac{\partial K'_i}{\partial K_j} \right|_{\mathbf{K}^*} \quad (2.279)$$

is evaluated at the non-trivial fixed point \mathbf{K}^* . The matrix $\mathbf{M}(b)$ is the so-called linearised renormalisation group transformation in the vicinity of the

Universality

fixed point \mathbf{K}^* .

Comparing Equation (2.277) with Equation (2.278), we identify that, to first order in $\delta\mathbf{K}$, the deviation from the fixed point after renormalisation $\delta\mathbf{K}'$ is related to the original deviation from the fixed point $\delta\mathbf{K}$ via the matrix $\mathbf{M}(b)$:

$$\delta\mathbf{K}' = \mathbf{M}(b)\delta\mathbf{K}. \quad (2.280)$$

For the i th entry $\delta K'_i$, Equation (2.280) implies that

$$\begin{aligned}\delta K'_i &= \sum_j [\mathbf{M}(b)]_{ij} \delta K_j \\ &= \sum_j \frac{\partial K'_i}{\partial K_j} \Big|_{\mathbf{K}^*} \delta K_j.\end{aligned} \quad (2.281)$$

Hence, the matrix $\mathbf{M}(b)$ determines the speed of the flow towards or away from the fixed point. The real matrix $\mathbf{M}(b)$ is not necessarily symmetric. For simplicity, however, we assume that $\mathbf{M}(b)$ is symmetric to guarantee that its eigenvalues are real and that the associated set of eigenvectors are orthogonal and form a convenient basis in which to discuss the flow. The aim is to investigate the flow in the coupling space along the eigenvectors of $\mathbf{M}(b)$. This will allow us to make simple but far reaching conclusions about the nature of the flow.¹³

To investigate the flow in detail, we introduce the eigenvalues, $\lambda_i(b)$, and the eigenvectors $\mathbf{e}_i(b)$ of the matrix $\mathbf{M}(b)$:

$$\mathbf{M}(b)\mathbf{e}_i(b) = \lambda_i(b)\mathbf{e}_i(b). \quad (2.282)$$

The eigenvectors $\{\mathbf{e}_i(b)\}$ are normalised and orthogonal

$$\mathbf{e}_i(b) \cdot \mathbf{e}_j(b) = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases} \quad (2.283)$$

and form a basis for the infinite-dimensional coupling space. We further assume that this basis is complete, that is, every point in the infinite-dimensional coupling space can be written as a linear combination of $\{\mathbf{e}_i(b)\}$.

Universality

We next define the (scalar) scaling field, u_i , as the length of the projection of the deviation from the fixed point along the direction of $\mathbf{e}_i(b)$:

$$u_i = \mathbf{e}_i(b) \cdot \delta \mathbf{K}, \quad (2.284)$$

such that the component of $\delta \mathbf{K}$ in the direction of $\mathbf{e}_i(b)$ is $[\mathbf{e}_i(b) \cdot \delta \mathbf{K}] \mathbf{e}_i(b)$ and therefore we may write

$$\begin{aligned} \delta \mathbf{K} &= \sum_{i=1}^{\infty} [\mathbf{e}_i(b) \cdot \delta \mathbf{K}] \mathbf{e}_i(b) \\ &= \sum_{i=1}^{\infty} u_i \mathbf{e}_i(b). \end{aligned} \quad (2.285)$$

We will shortly be able to identify the scaling fields with reduced control parameters, such as the reduced temperature, reduced external field and so on. Hence, as experimenters we can control the initial value of the scaling fields.

The renormalised scaling field, u'_i , is the projection of the deviation from the fixed point along the direction of $\mathbf{e}_i(b)$ after renormalisation. Using the expansion in Equation (2.285) of $\delta \mathbf{K}$ along the directions of the eigenvectors, we can relate the transformed scaling field to the original scaling field:

$$\begin{aligned} u'_i &= \mathbf{e}_i(b) \cdot \delta \mathbf{K}' \\ &= \mathbf{e}_i(b) \cdot \mathbf{M}(b) \delta \mathbf{K} \\ &= \mathbf{e}_i(b) \cdot \mathbf{M}(b) \sum_{j=1}^{\infty} u_j \mathbf{e}_j(b) \\ &= \mathbf{e}_i(b) \cdot \sum_{j=1}^{\infty} u_j \mathbf{M}(b) \mathbf{e}_j(b) \\ &= \mathbf{e}_i(b) \cdot \sum_{j=1}^{\infty} u_j \lambda_i(b) \mathbf{e}_j(b) \\ &= \lambda_i(b) u_i, \end{aligned} \quad (2.286)$$

where in the last step we have made use of the orthonormality of the eigenvectors, see Equation (2.283). Hence, the transformed scaling field is related to the original scaling field by the factor $\lambda_i(b)$, which is the eigenvalue of $\mathbf{M}(b)$ associated with the eigenvector in the direction $\mathbf{e}_i(b)$.

Universality

Now, from the semi-group property of the renormalisation group transformation in Equation (2.266) it follows that

$$\mathbf{M}(b_2)\mathbf{M}(b_1) = \mathbf{M}(b_2 b_1), \quad (2.287)$$

implying that the eigenvalues satisfy the condition

$$\lambda_i(b_2)\lambda_i(b_1) = \lambda_i(b_2 b_1). \quad (2.288)$$

The unique solution of the functional equation in Equation (2.288) is a power law, such that

$$\lambda_i(b) = b^{y_i}, \quad (2.289)$$

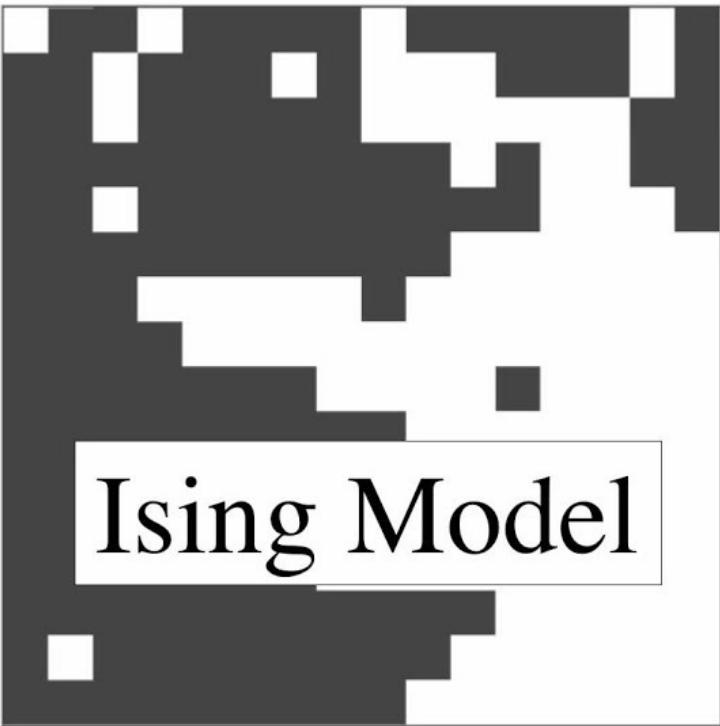
where y_i are the so-called renormalisation group eigenvalues. Substituting Equation (2.289) into Equation (2.286) we arrive at our principle result

$$u'_i = b^{y_i} u_i. \quad (2.290)$$

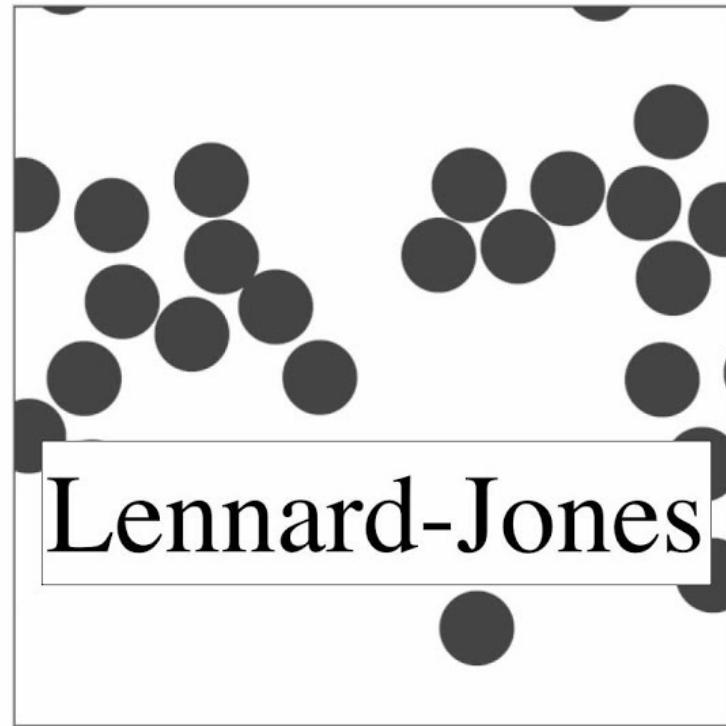
The derivation of the relation in Equation (2.290) between the renormalised and original scaling field puts the heuristic assumptions in Equation (2.218) of the Kadanoff block spin transition on a firm mathematical footing.

The factor b^{y_i} determines whether the scaling field increases, decreases or remains constant under renormalisation. We may distinguish three different cases:

- *Relevant scaling field.* If $y_i > 0$, then $\lambda_i(b) = b^{y_i} > 1$. The deviation from the fixed point along the direction of $e_i(b)$ increases upon renormalisation. The scaling field u_i with $y_i > 0$ is said to be relevant, since the renormalisation group flow is driven away from the non-trivial fixed point. A relevant scaling field eventually explodes upon application of the renormalisation group transformation.
- *Irrelevant scaling field.* If $y_i < 0$, then $\lambda_i(b) = b^{y_i} < 1$. The deviation from the fixed point along the direction of $e_i(b)$ decreases upon renormalisation. The scaling field u_i with $y_i < 0$ is said to be irrelevant, since the renormalisation group flow is driven towards the non-trivial fixed point. An irrelevant scaling field eventually vanishes upon application of the renormalisation group transformation.
- *Marginal scaling field.* If $y_i = 0$, then $\lambda_i(b) = b^{y_i} = 1$. The scaling field u_i with $y_i = 0$ is said to be marginal. A first order Taylor expansion in $\delta\mathbf{K}$ is insufficient to determine whether the flow is directed towards or away from the fixed point.



Ising Model



Lennard-Jones

Widom scaling

$$\begin{aligned}
Z(\mathbf{K}, N) &= \sum_{\{s_i\}} \exp(-\beta E_{\{s_i\}}) \\
&= \sum_{\{s_I\}} \sum_{\substack{\text{configurations } \{s_i\} \\ \text{consistent with } \{s_I\}}} \exp(-\beta E_{\{s_i\}}) \\
&= \exp(N' K'_0) \sum_{\{s_I\}} \exp(-\beta E'_{\{s_I\}}) \\
&= \exp(N' K'_0) Z(\mathbf{K}', N'). \tag{2.292}
\end{aligned}$$

Meanwhile, since the number of spins is reduced to $N' = N/b^d$, the free energy per spin transforms according to

$$\begin{aligned}
f(\mathbf{K}) &= -\frac{1}{N} k_B T \ln Z(N, \mathbf{K}) \\
&= -b^{-d} \frac{1}{N'} k_B T [N' K'_0 + \ln Z(N', \mathbf{K}')] \\
&= f_r(\mathbf{K}) + b^{-d} f_s(\mathbf{K}'). \tag{2.293}
\end{aligned}$$

We identify the term arising from the renormalised constant coupling K'_0 as the regular part of the free energy per spin¹⁴ $f_r(\mathbf{K})$. Therefore, the free energy per spin transforms inhomogeneously. However, the singular part of the free energy per spin transforms as a generalised homogeneous function according to

$$f_s(\mathbf{K}) = b^{-d} f_s(\mathbf{K}'). \tag{2.294}$$

Although coupling constants involving K_0 , renormalised or otherwise, do not appear in the probability distribution of microstates, they are nevertheless required for the correct transformation of the free energy per spin. To see this, we argue that Equation (2.294) alone cannot be valid: Assume, for the moment, that (2.294) is a valid transformation for the free energy per spin. Then, at the non-trivial fixed point $f(\mathbf{K}^*) = b^{-d} f(\mathbf{K}^*)$, implying that $f(\mathbf{K}^*) = 0$ or $f(\mathbf{K}^*) = \infty$. The latter is not physical and the former cannot be true in general. Equation (2.294) only pertains to the singular part of the free energy, which indeed takes the value $f_s(\mathbf{K}^*) = 0$, but with derivatives that are diverging [Wilson, 1971a].

Widom scaling

Close to the fixed point on the critical surface it is convenient to use the eigenvectors of \mathbf{M} as the basis. Since the scaling fields are the deviations of \mathbf{K} from the fixed point, we find that after applying the renormalisation group transformation n times

$$\begin{aligned} f_s(t, h, u_3, u_4, \dots) &= b^{-d} f_s(b^{y_t} t, b^{y_h} h, b^{y_3} u_3, b^{y_4} u_4, \dots) \\ &= b^{-nd} f_s(b^{ny_t} t, b^{ny_h} h, b^{ny_3} u_3, b^{ny_4} u_4, \dots). \end{aligned} \quad (2.295)$$

In the limit of $n \rightarrow \infty$ all the irrelevant scaling fields u_3, u_4, \dots : iterate to zero and

$$f_s(t, h, u_3, u_4, \dots) = b^{-nd} f_s(b^{ny_t} t, b^{ny_h} h, 0, 0, \dots). \quad (2.296)$$

However, we would like to express the transformation in Equation (2.296) in a form that does not explicitly refer to the arbitrary scale factor b . Therefore, choosing $b^{ny_t} = |t|^{-1}$ we find

$$\begin{aligned} f_s(t, h, u_3, u_4, \dots) &= |t|^{d/y_t} f_s(t/|t|, h/|t|^{y_h/y_t}, 0, 0, \dots) \\ &= |t|^{d/y_t} f_s(\pm 1, h/|t|^{y_h/y_t}, 0, 0, \dots) \\ &= |t|^{d/y_t} \mathcal{F}_\pm(h/|t|^{y_h/y_t}). \end{aligned} \quad (2.297)$$

Hence, we have derived the Widom scaling ansatz in the general formalism developed by Wilson. In principle, the eigenvalues and eigenvectors of the renormalisation group transformation can be determined and hence critical exponents calculated, see Exercise 2.8.

Landau's school

- In Kharkiv, he and his friend and former student, Evgeny Lifshitz, began writing the *Course of Theoretical Physics*, ten volumes that together span the whole of the subject and are still widely used as graduate-level physics texts.
- Landau developed a famous comprehensive exam called the "Theoretical Minimum" which students were expected to pass before admission to the school. The exam covered all aspects of theoretical physics, and between 1934 and 1961 only 43 candidates passed, but those who did later became quite notable theoretical physicists.

