4.3 Second order transition — an example

4.3.1 The ferromagnet

- Ferromagnetism: below a certain temperature a magnetisation will spontaneously appear in the absence of an applied magnetic field.
- The interaction responsible for ferromagnetism is the *exchange interaction* between electron spins.
- Origin of the exchange interaction is the necessity to antisymmetrise the electronic wavefunction, together with the Coulomb repulsion between electrons.
- Then the symmetric and the antisymmetric wavefunctions have different energies.

- . . .symmetric and the antisymmetric wavefunctions have different energies.

- This may be written as an *effective* spin-dependent hamiltonian:

$$\mathscr{H}_{\mathrm{x}} = -\hbar J \sum_{ij}^{\mathrm{nn}} \mathbf{S}_i \cdot \mathbf{S}_j \,.$$

  This is called the *Heisenberg exchange* hamiltonian. — Should be familiar from Atomic Physics.

- When J is positive the energy is minimised when the spins are *parallel*; this is the energetically favourable state $\Longrightarrow$ *ferromagnetism*.

  (When J is negative the energy is minimised when the spins are *antiparallel*; this is the energetically favourable state $\Longrightarrow$ *antiferromagnetism)*.

Symmetry breaking

- The exchange hamiltonian is *rotationally invariant*.
- The magnetisation, when it appears, points in a *specific direction*.

- Thus the ferromagnetic transition breaks *rotational symmetry*.

Phase diagram

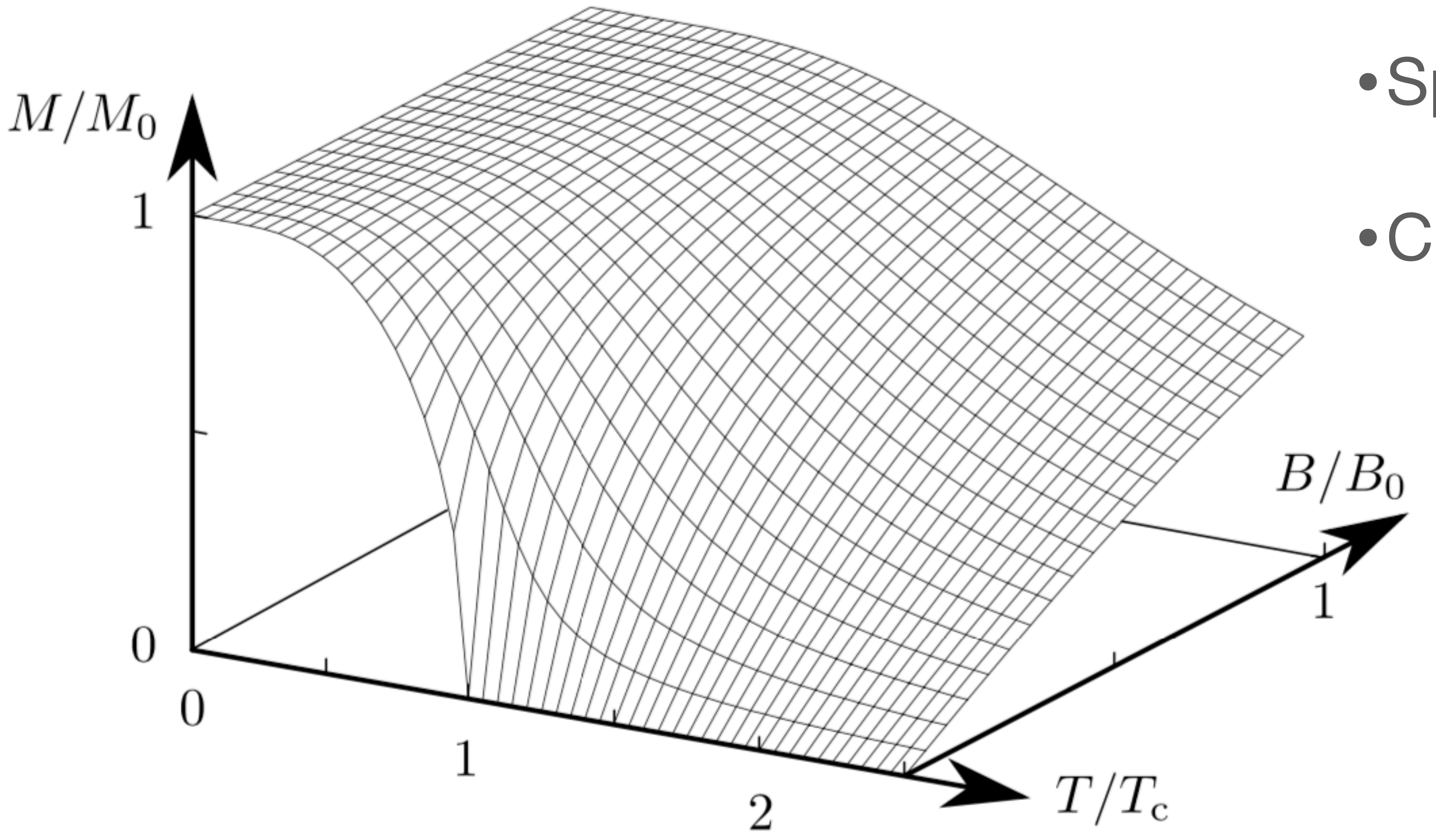

Figure 4.15: Phase diagram for a magnetic system.

- Paramagnetism
- Spontaneous magnetisation
- Critical point

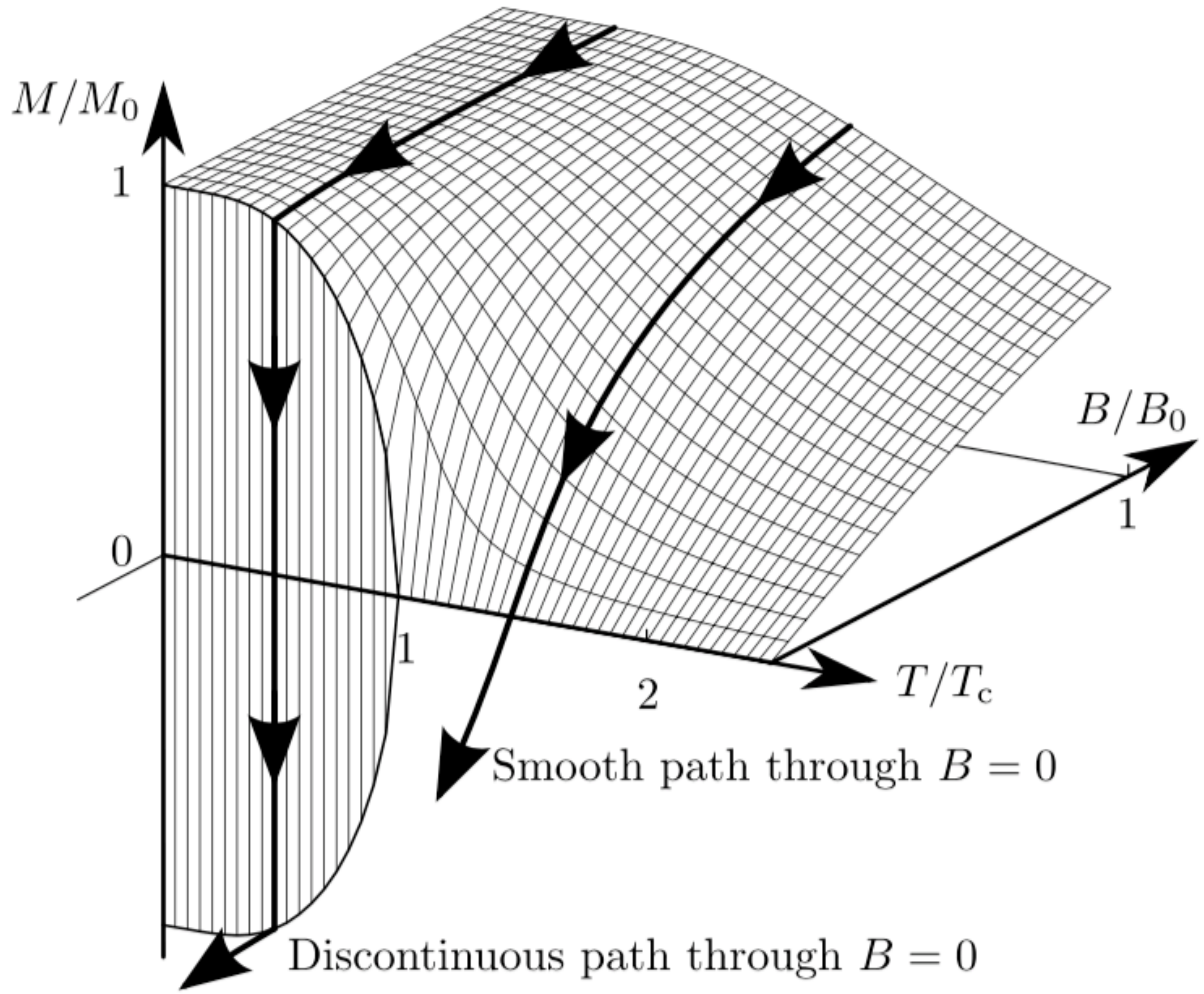

Figure 4.16: Variation of M as B goes through zero.

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4.3.2 The Weiss model

- The behaviour of the ferromagnet is contained in its hamiltonian.
- Apply a magnetic field (in the z direction)

$$\mathscr{H} = -\hbar\gamma \mathbf{B} \cdot \sum_i \mathbf{S}_i - \hbar J \sum_{ij}^{\mathrm{nn}} \mathbf{S}_i \cdot \mathbf{S}_j$$

first term is usual $-\mathbf{M} \cdot \mathbf{B}$ Zeemain interaction. ($\mathbf{M} = \hbar\gamma \sum_i \mathbf{S}_i$)

- Can write $\mathscr{H}$ as

$$\mathscr{H} = -\hbar\gamma \left\{ \mathbf{B} + \frac{J}{\gamma} \sum_j^{\mathrm{nn}} \mathbf{S}_j \right\} \cdot \sum_i \mathbf{S}_i$$

Weiss local field

- Each spin sees the applied $\mathbf{B}$ field plus an extra (exchange) field from its neighbours

$$\mathbf{b}_i = \frac{J}{\gamma} \sum_j^{\mathrm{nn}} \mathbf{S}_j$$

  the sum is over all spins neighbouring i.

- The $\mathbf{b}_i$ will be different at different sites, and varying with time.

- Weiss (1907) approximated the fields to be the same and constant.

$$\mathbf{b} = \frac{J}{\gamma} \left\langle \sum_j^{\mathrm{nn}} \mathbf{S}_j \right\rangle = nJ\langle \mathbf{S} \rangle / \gamma = \frac{nJ}{N\gamma^2 \hbar} \mathbf{M}.$$

Equation of state

- Equation of state for a *paramagnet*:

$$M = N\frac{\gamma\hbar}{2}\tanh\frac{\gamma\hbar B}{2kT} \qquad \text{(}\mathbf{M}\text{ and }\mathbf{B}\text{ parallel)}$$

- Weiss recipe: wherever you had B, you now put $B + b$; $\quad b = \dfrac{nJ}{N\gamma^2\hbar}M$

- giving

$$M = N\frac{\gamma\hbar}{2}\tanh\frac{\gamma\hbar}{2kT}\left\{B + \frac{nJ}{N\gamma^2\hbar}M\right\}.$$

- *Implicit* equation relating M, B and T.

4.3.3 Spontaneous magnetisation

- *Spontaneous* magnetisation means magnetisation that appears in the *absence* of a magnetic field, as temperature is reduced.

  T at which this occurs is the critical temperature T_c.

- So put $B = 0$ in the equation of state:

$$M = N\frac{\gamma\hbar}{2}\tanh\left\{\frac{nJ}{2kTN\gamma}M\right\}.$$

Still a nonlinear and implicit equation. (M is what we *want*; it has no business being on the right hand side.)

Two different ways of solution . . . . . .

Graphical solution

- Want to solve

$$M = N\frac{\gamma\hbar}{2}\tanh\left\{\frac{nJ}{2kTN\gamma}M\right\}$$

for M as a function of T.

- Define auxiliary quantity X:

$$X = \frac{nJ}{2kTN\gamma}M$$

gives simultaneous equations:

$$\left.\begin{aligned} M &= N\frac{\gamma\hbar}{2}\tanh X \\ M &= \frac{2kTN\gamma}{nJ}X\,. \end{aligned}\right\} \quad \text{Solve graphically}$$

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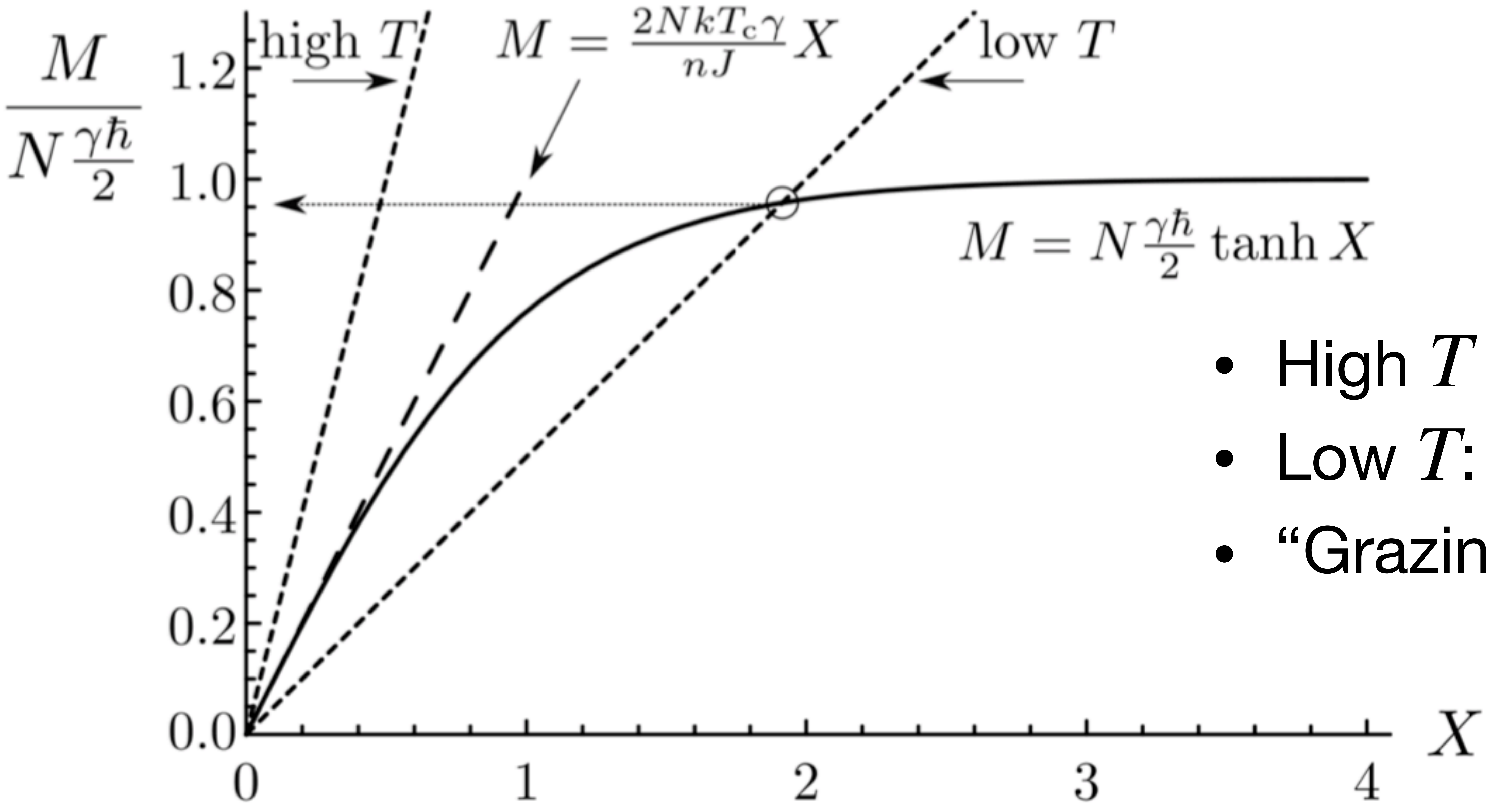


Figure 4.17: Graphical solution for spontaneous magnetization.

- High T : solution $M = 0$
- Low T: solution for finite M
- "Grazing" solution at $T = T_\mathrm{c}$

$$T_\mathrm{c} = \frac{\hbar n}{4k}J$$

Smart-ass solution

- Can't solve

$$M = N\frac{\gamma\hbar}{2}\tanh\left\{\frac{nJ}{2kTN\gamma}M\right\}$$

  for M as a function of T.
  – But can solve for T as a function of M.

- In terms of *saturation magnetisation* $M_0 = N\gamma\hbar/2$
  and *critical temperature* $T_\mathrm{c} = \hbar nJ/4k$

gives
$$\frac{M}{M_0} = \tanh\left\{\frac{M}{M_0}\frac{T_\mathrm{c}}{T}\right\}$$
very neat!!

- $$\frac{M}{M_0} = \tanh\left\{\frac{M}{M_0}\frac{T_c}{T}\right\}$$

  can be "solved"

  $$\frac{M}{M_0}\frac{T_c}{T} = \tanh^{-1}\left(\frac{M}{M_0}\right) = \frac{1}{2}\ln\left(\frac{1+M/M_0}{1-M/M_0}\right)$$

  so that

  $$\frac{T}{T_c} = \frac{2M/M_0}{\ln\left[(1+M/M_0)\big/(1-M/M_0)\right]}.$$

Spontaneous magnetisation as a function of temperature

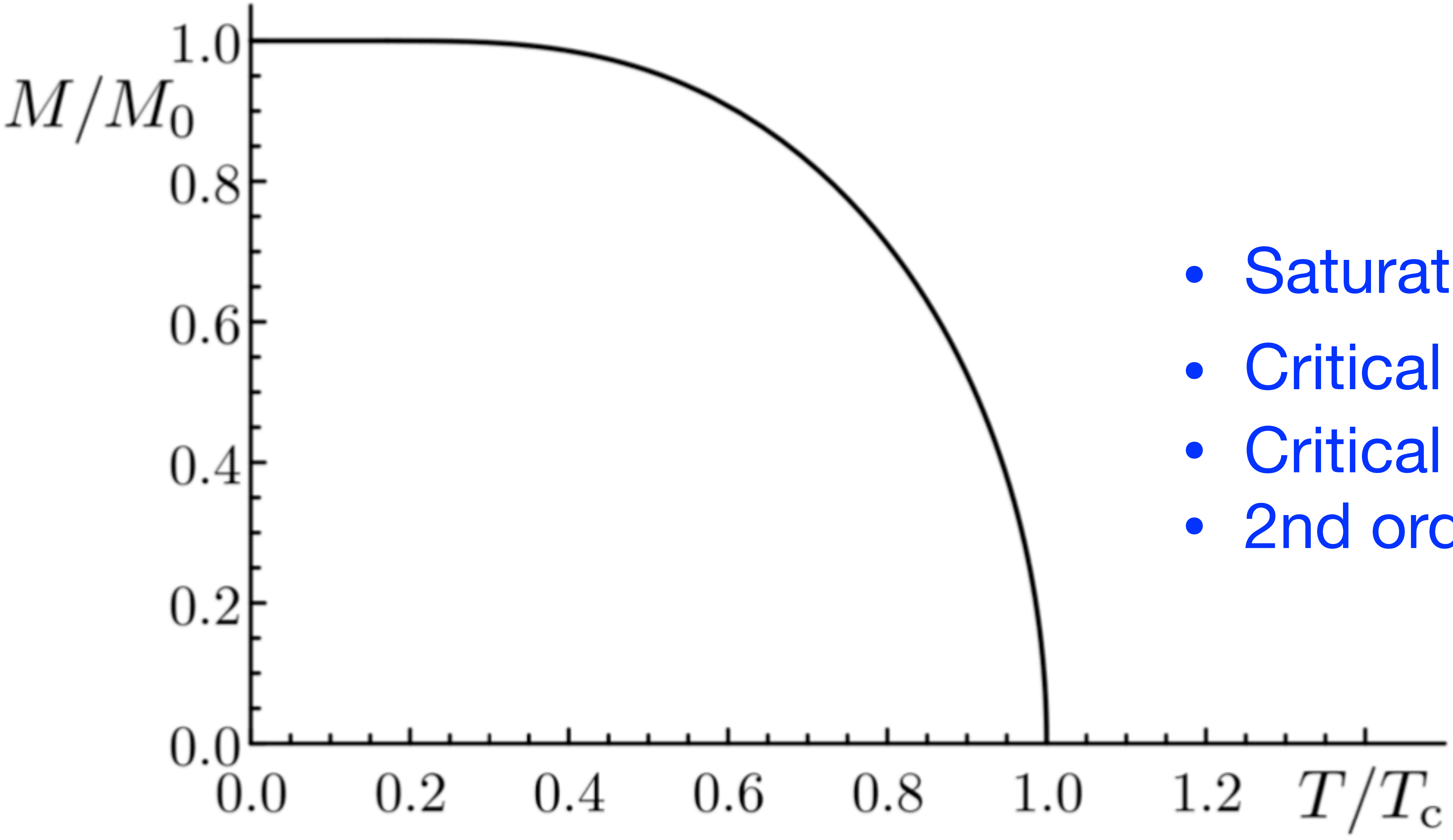
- 

Figure 4.18: Spontaneous magnetization of a ferromagnet.

- Saturation magnetisation M_0
- Critical temperature T_c
- Critical point
- 2nd order transition

4.3.4 Critical behaviour — Universality (Ising class)

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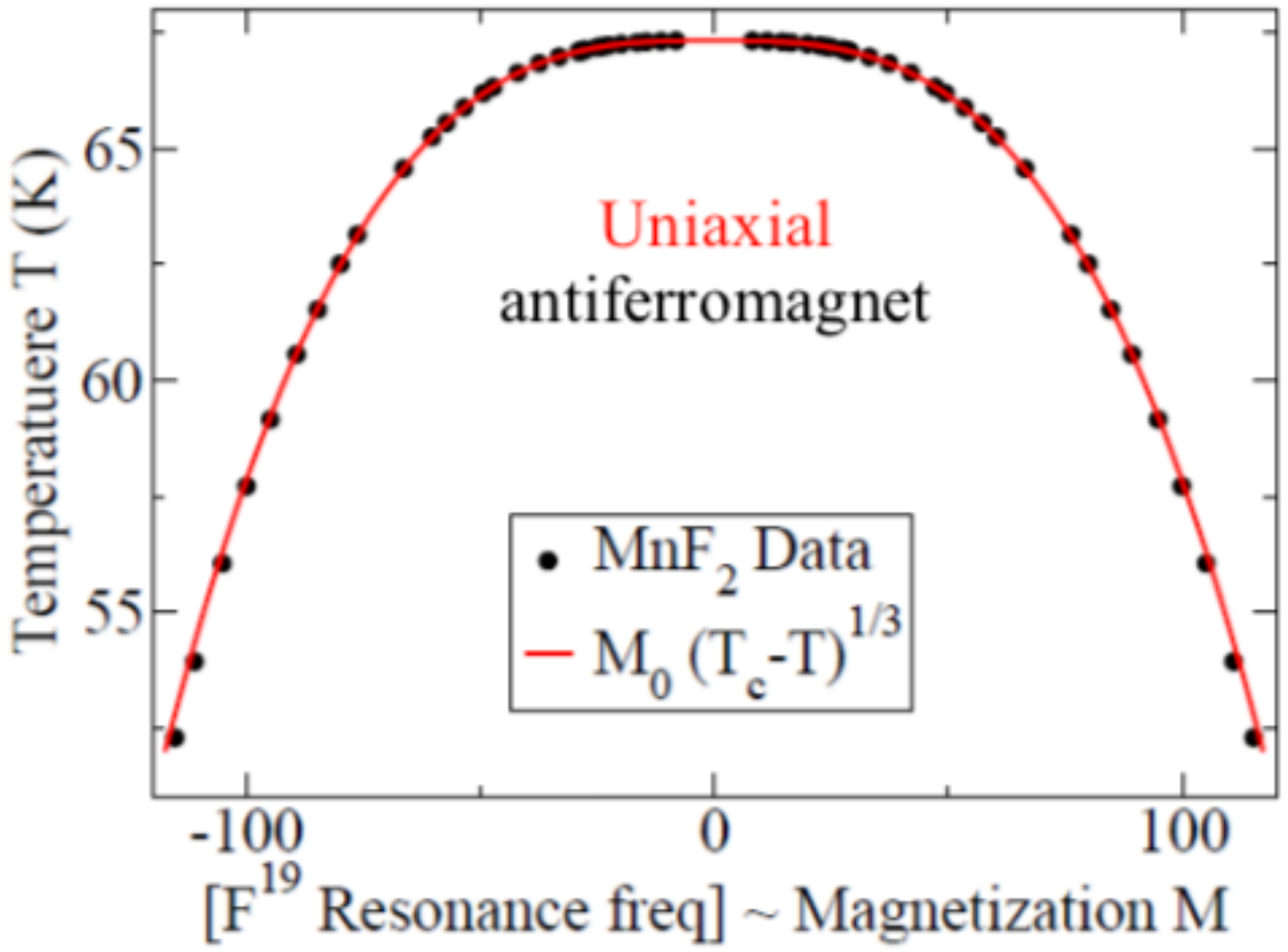

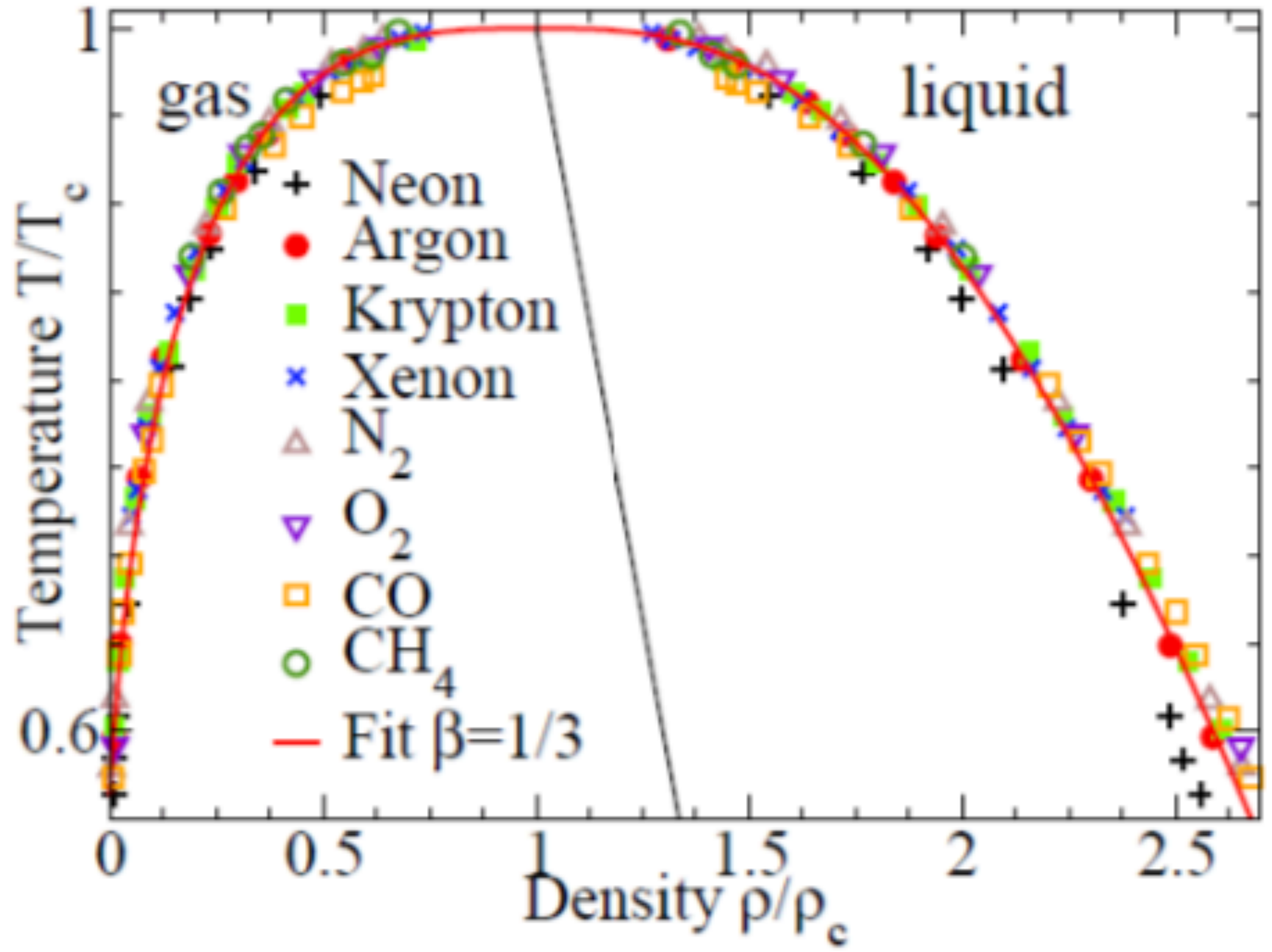

Fig. 12.8 Universality: Ferromagnetic-Paramagnetic Critical Point. Magnetization versus temperature for a uniaxial antiferromagnet MnF_2 [64]. We've shown both branches $\pm M(T)$ and swapped the axes so as to make the analogy with the liquid–gas critical point apparent (figure 12.7). Notice that both the magnet and the liquid–gas critical point have order parameters that vary as $(1 - T/T_c)^\beta$ with $\beta \approx 1/3$. (The liquid–gas coexistence curves are tilted: the two theory curves would align if we defined an effective magnetization for the liquid gas critical point $\rho_{\text{eff}} = \rho - 0.75\rho_c(1 - T/T_c)$ (thin midline, figure 12.7).) This is not an accident: both are in the same universality class, along with the three-dimensional Ising model, with the current estimate for $\beta = 0.325 \pm 0.005$ [170, Chapter 28].

Fig. 12.7 Universality: Liquid–Gas Critical Point. The liquid–gas coexistence lines ($\rho(T)/\rho_c$ versus T/T_c) for a variety of atoms and small molecules, near their critical points (T_c, ρ_c) [61]. The curve is a fit to the argon data, $\rho/\rho_c = 1 + s(1 - T/T_c) \pm \rho_0(1 - T/T_c)^\beta$ with $s = 0.75$, $\rho_0 = 1.75$, and $\beta = 1/3$ (reference [61]).

-- James P. Sethna, Entropy, Order Parameters, and Complexity

Critical behaviour (behaviour in the vicinity of the critical point)

- Close to the CP, M is small. So from

$$\frac{M}{M_0} = \tanh\left\{\frac{M}{M_0}\frac{T_c}{T}\right\}$$

we can expand the tanh: $\left(\tanh x = x - x^3/3 + \ldots\right)$

$$\frac{M}{M_0} = \frac{M}{M_0}\frac{T_c}{T} - \frac{1}{3}\left(\frac{M}{M_0}\frac{T_c}{T}\right)^3 + \ldots$$

- This can be re-arranged to give

$$\frac{M}{M_0} = \pm\sqrt{3}\frac{T}{T_c}\left(1 - \frac{T}{T_c}\right)^{1/2} + \ldots$$

- From

$$\frac{M}{M_0} = \pm\sqrt{3}\frac{T}{T_c}\left(1 - \frac{T}{T_c}\right)^{1/2} + \ldots$$

So close to CP we have

$$\frac{M}{M_0} \sim \pm\sqrt{3}\left(1 - \frac{T}{T_c}\right)^{1/2}.$$

- The dominant, singular part of the behaviour is in the factor $(1 - T/T_c)^{1/2}$.
- The exponent $1/2$ is the critical exponent β introduced in Section 4.1.7.
- The coefficient of the singular part is the *critical amplitude* $b = \sqrt{3}$
- So the Weiss model gives a 2nd order transition with $\beta = 1/2$ and $a = \sqrt{3}$.

4.3.5 Magnetic susceptibility

- For a non-interacting paramagnet

$$M = M_0 \tanh \frac{M_0 B}{NkT} .$$

- At high T or low B (whenever M/M_0 is small), can expand the tanh:

$$M = \frac{M_0^2}{NkT} B = \frac{C}{T} B.$$

- The *magnetic susceptibility* χ is defined

$$\chi = \frac{\mu_0}{V}\frac{M}{B}.$$

$$\left.\begin{matrix} M = \frac{M_0^2}{NkT} B = \frac{C}{T} B \\ \chi = \frac{\mu_0}{V}\frac{M}{B} \end{matrix}\right\} \quad \chi = \frac{\mu_0}{V}\frac{C}{T}$$

Incorporating b

- We *had*

$$M = \frac{C}{T} B \quad \text{equivalently} \quad \chi = \frac{\mu_0}{V}\frac{C}{T}$$

- Now follow the Weiss prescription $B \to B + b$, where

$$b = \frac{NkT_c}{M_0} M = \frac{T_c}{C} M$$

so that

$$M = \frac{C}{T} B + \frac{T_c}{T} M\,,$$

or

$$M = \frac{C}{T - T_c} B \quad \text{equivalently} \quad \chi = \frac{\mu_0}{V}\frac{C}{T - T_c}$$

Curie law and Curie-Weiss law

- Non-interacting spins

$$\chi = \frac{\mu_0}{V}\frac{C}{T}$$

$\chi \propto 1/T$ called Curie's law.

- Interacting spins

$$\chi = \frac{\mu_0}{V}\frac{C}{T - T_c}$$

called Curie-Weiss law.

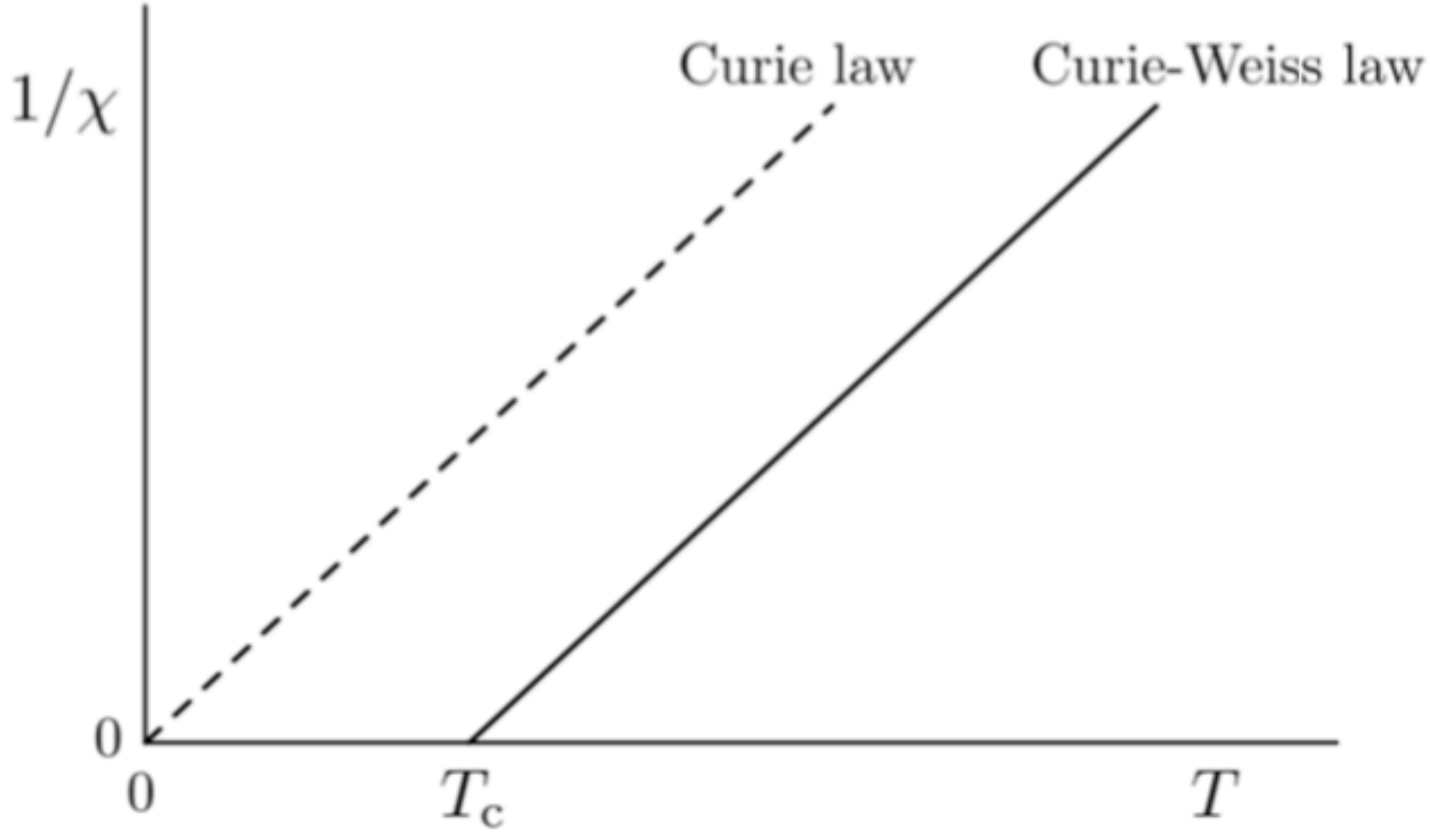

Figure 4.19: Curie and Curie-Weiss laws.

- Exponent γ: $\chi \sim (T - T_c)^{-\gamma}$, so Weiss model gives $\gamma = 1$

4.3.6 The ground state and Goldstone modes

Ground states

- Below a critical temperature a spontaneous magnetisation appears.
- This happens in the absence of an applied magnetic field.
- The magnetisation appears in a completely arbitrary direction.
- The interaction responsible for the transition is the rotationally-invariant Heisenberg hamiltonian.
- But M must point in some direction.
- Thus the transition breaks the (rotational) symmetry of the hamiltonian.

- There is also the $M = 0$ solution — but this has *higher* energy.

- The ground state ($M \neq 0$) has many possible directions.

- I.e the ground state is *highly degenerate*.

- Denote the set of degenerate ground states by $\left|\hat{\mathbf{r}}\right\rangle$ where $\hat{\mathbf{r}}$ is the direction of the magnetisation.

Figure 4.20: Different possible ground states.

- One *always* observes one of the $\left|\hat{\mathbf{r}}\right\rangle$ states; never a linear superposition of these states, even this is allowed by the laws of quantum mechanics.

– – –Paradox – – –

- This is essentially the paradox of Schrödinger's cat.

Goldstone modes

- The ground state corresponds to a uniform order parameter; the magnetisation points in the same direction throughout the specimen.

- It costs energy to deform the order parameter (make it non-uniform)

- So consider a sinusoidal spatially varying order parameter $\mathbf{M}(\mathbf{r})$:

$$\mathbf{M}(\mathbf{r}) = M_0 \left\{ \cos(\mathbf{k}\cdot\mathbf{r})\hat{\mathbf{x}} + \sin(\mathbf{k}\cdot\mathbf{r})\hat{\mathbf{y}} \right\}.$$

- This has an energy above that of the ground state.

- This is the spatial part of a spin wave with wave vector $\mathbf{k}$.

- In the limit $\mathbf{k} \to 0$ this reduces to the ground state.

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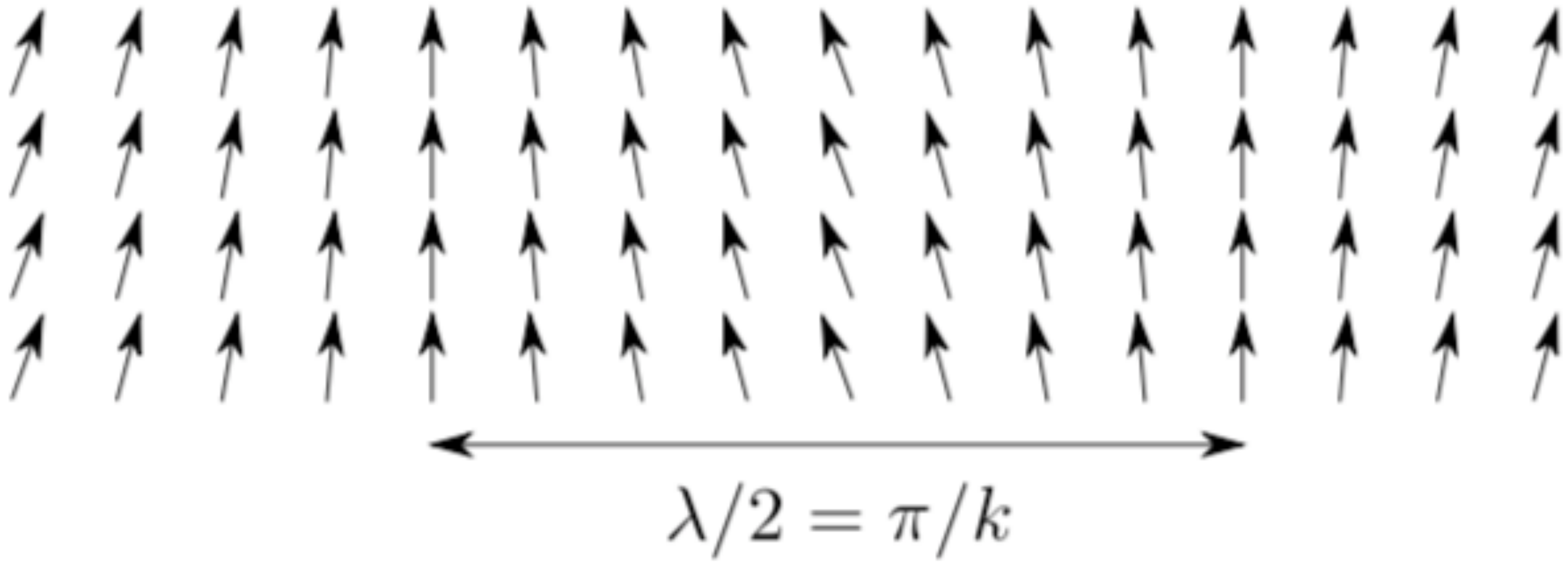


- In the limit $\mathbf{k} \to 0$ this reduces to the ground state.

- This is the physical content of **Goldstone's theorem**:

  when a continuous symmetry is broken there will be excitations involving variations in the order parameter and the dispersion relation for these excitations satisfies
  $$\varepsilon(k) \to 0 \quad \text{as} \quad k \to 0.$$

- These excitations are known as *Goldstone modes* or, when quantized, as *Goldstone bosons*. They are the low energy excitations and thus they determine the low temperature thermal properties of a system.

- The fact that $\varepsilon(k)$ goes to zero *continuously* means that there is no energy gap between the ground state and the excitations. This may also be interpreted as saying that the Goldstone bosons have *zero mass*.

- Goldstone's theorem follows only when the interaction responsible for the symmetry breaking is of short range. We may contrast this with the superconducting transition. There the long range of the Coulomb force results in a gap in the plasmon excitation spectrum; then the bosons *have mass*. This is the condensed matter analogue of the Higgs mechanism elementary particles acquire mass.

4.4 The Ising and other models

History and motivation

- Interactions are responsible for phase transitions.
- But many interactions are complicated — so you can’t actually calculate.

  — Either . . System is simple/calculable — does nothing interesting
  — or . . it is complex/un-calculable — but behaves interestingly.

- Challenge: find the simplest interaction that does something interesting (phase transition) but is simple enough that you can calculate with it.
- This was taken up by Wilhelm Lenz and his student Ernst Ising.

- Heisenberg hamiltonian

$$\mathscr{H}_{\mathrm{x}} = -\hbar J \sum \mathbf{S}_i \cdot \mathbf{S}_j$$
$$= -\hbar J \sum \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right).$$

- Can we simplify? Lenz suggested to Ising: just take the z bit.

- The interaction

$$\mathscr{H}_{\mathrm{I}} = -\hbar J \sum S_i^z S_j^z$$

is called the Ising hamiltonian.

Specifically for spin $\frac{1}{2}$

i.e. *two* states.

But my non-standard notation!

- Problem: Does this interaction result in a phase transition?

(microscopic — first principles calculation)

(Think back — the Weiss arguments would apply equally to the Ising case.)

- Ising 1920 solved the problem (in 1d):

  there was no phase transition.

  But he couldn't do 2d and higher.

- Onsager 1944 solved the 2d problem:

  there was a phase transition at finite T.

- No one has managed to solve the 3d case. Probably impossible.

  By *solve* one means (at least) an analytical expression for T_c as a function of J.

Ubiquity of the Ising model

- There are particles/spins arranged on a regular lattice.
- The particle/spin on each site will be in one of two possible states.
- If the states are “spin up” or “spin down” then the model describes a magnet.
- A lattice gas would have states “atom present” and “no atom present”.
- A binary alloy would have states “A atom on site” and “B atom on site”.
- The interaction is between neighbours: it has one value if the neighbouring states are the same and another if the states are different. The energy *difference* is the characteristic energy of the model.

4.4.3 Ising model in 1d

- Remember — Ising found no transition (no spontaneous magnetisation).
- He calculated (complicated) the partition function, and from that:

$$m = \frac{\sinh \gamma\hbar B/kT}{\sqrt{\sinh \gamma\hbar B/kT + e^{-\hbar J/kT}}}$$

— see Plische and Bergersen.

- When $B = 0$ there is no magnetisation at any temperature, except $T = 0$.
- But when $B \neq 0$, at low temperature, will get the saturation magnetisation.

Landau's demonstration

- Chain of N spins

- Reverse spins from one point onwards (a "kink").
- Energy: the kink increases energy by $\hbar J$ (no applied field).
- Entropy: choice of N sites for kink. So the kink increases S by $k \ln N$.
- $\implies$ Kink increases free energy $F = E - TS$ by

$$\Delta F = \hbar J - kT \ln N.$$

- $$\Delta F = \hbar J - kT \ln N$$
- Equilibrium state minimises F.

  — Kink *increases* energy contribution by $\hbar J$
  — but *decreases* entropy contribution by $kT \ln N$.

- In the thermodynamic limit ($N \to \infty$) the entropy term will win.
- So a kink will *reduce* the free energy - so it is favoured.
- So the ordered state cannot be the thermodynamically favoured state.

  i.e. in 1d there will not be a transition to the ordered state.

Brilliant !!!!!!!

4.4.3 Ising model in 2d

- Onsager (1944) found there was a transition for the Ising model in 2d.

- He calculated

$$F = -Nk\ln\left(2\cosh \hbar J/2kT\right) - \frac{Nk}{2\pi}\int_0^{\infty} \ln\frac{1}{2}\left(1+\sqrt{1+\kappa^2\sin^2\varphi}\right)\mathrm{d}\varphi$$

where

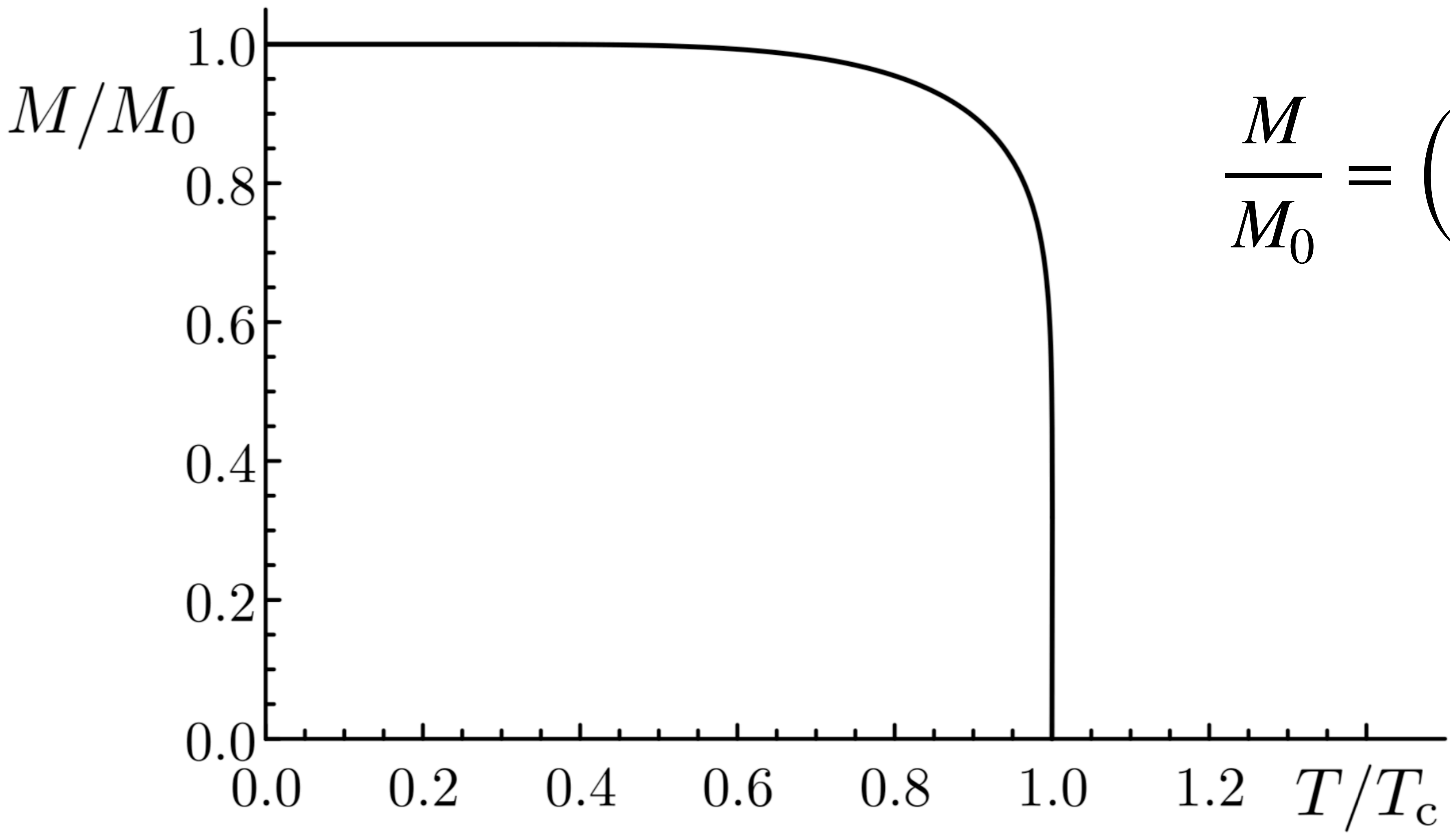
$$\kappa = \frac{2}{\cosh \hbar J/2kT \, \coth \hbar J/2kT}\,.$$

Singularity in F occurs at solution to

$$\sinh \hbar J/2kT_\mathrm{c} = 1 \quad \text{or} \quad T_\mathrm{c} = \frac{1}{2\ln\left(1+\sqrt{2}\right)}\frac{\hbar J}{k} \quad \text{or} \quad T_\mathrm{c} = 0.567\hbar J/k\,.$$

- (fractional) magnetisation

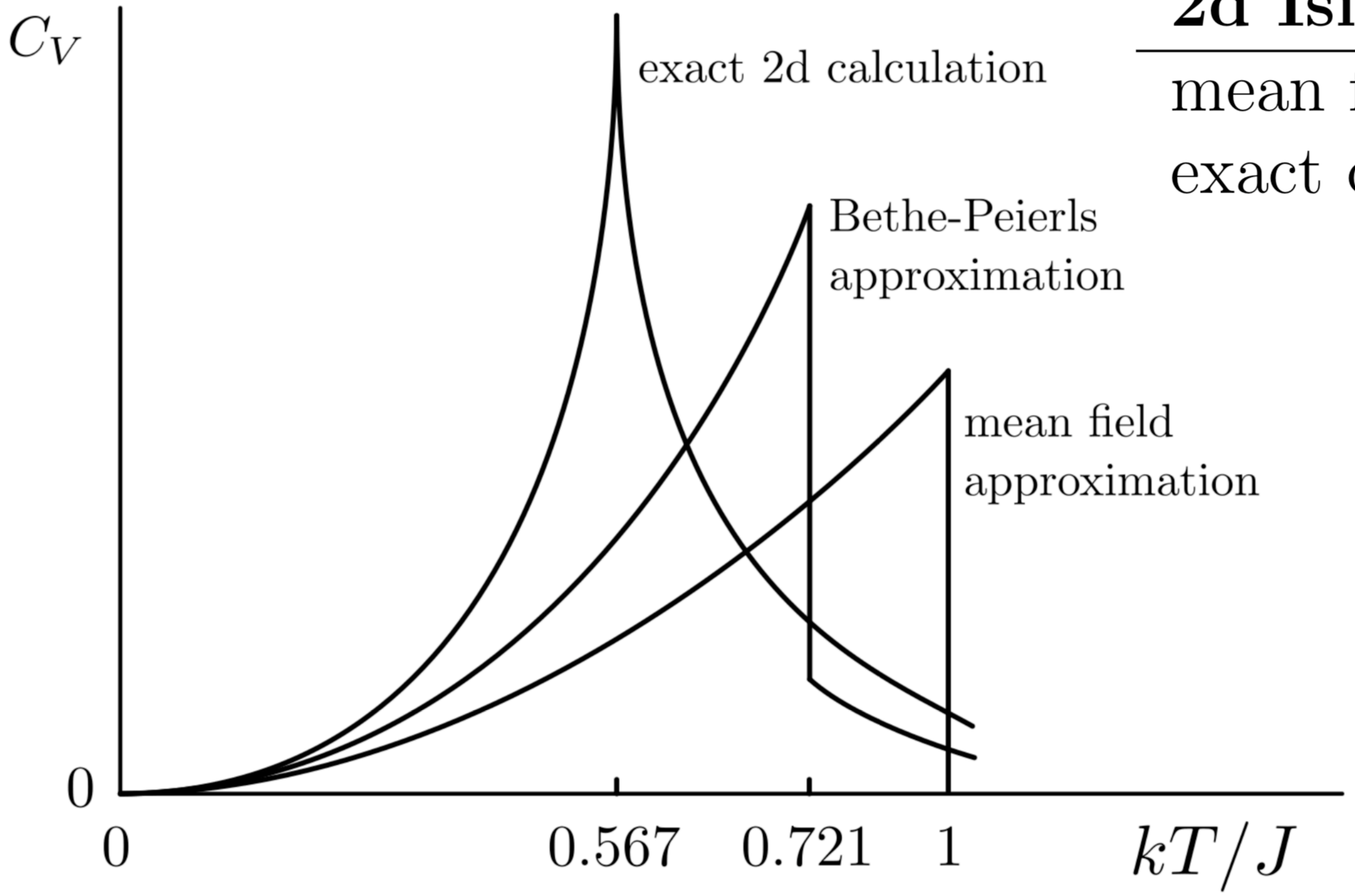
$$\frac{M}{M_0} = \left\{ 1 - \left(\sinh \hbar J / 2kT \right)^{-4} \right\}^{1/8}.$$



$$\frac{M}{M_0} = \left(4\sqrt{2}\ln\left(1+\sqrt{2}\right)\right)^{1/8}\left(\frac{T_c - T}{T_c}\right)^{1/8} + \dots$$

$$\beta = 1/8, \qquad b = 1.224$$

- Heat capacity ↓



Critical exponents ↓

2d Ising model	α	β	γ	δ	ν	η
mean field	0	½	1	3	½	0
exact calc.	0	⅛	7/4	15	1	0

$\boxed{\text{Mean field} \equiv \text{Weiss model} \quad \text{Mean field independent of } d}$

The XY model and the Spherical model

4.4.6 The XY model

- Heisenberg $$\mathscr{H}_{\mathrm{x}} = -\hbar J \sum \left(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right)$$
- XY $$\mathscr{H}_{\mathrm{xy}} = -\hbar J \sum \left(S_i^x S_j^x + S_i^y S_j^y \right)$$
- Ising $$\mathscr{H}_{\mathrm{I}} = -\hbar J \sum \left(S_i^z S_j^z \right)$$

- The order parameter for this model is the magnetization in the $x-y$ plane; it is a vector of dimension $n=2$.

- Thus the order parameter is two-dimensional.

- Since the magnetisation can point in any direction in the $x-y$ plane, it can vary *continuously*; the XY transition thus breaks a continuous symmetry.

- This model is regarded as a good description for the conventional superconducting transition and the superfluid transition in liquid ^{4}He, since the order parameter in this case is a two component vector (or a complex scalar).

- Estimates for critical exponents for the XY model in three spatial dimensions are given in the table in Section 4.9.3.

4.4.7 Spherical model

- Introduced by Marck Kac in 1952
- $$\mathscr{H}_{\mathrm{s}} = -\hbar J \sum \left(S_i^{\alpha} S_j^{\alpha} + S_i^{\beta} S_j^{\beta} + S_i^{\gamma} S_j^{\gamma} + \ldots + S_i^{D} S_j^{D} \right) \text{ as } D \to \infty$$
- It is an extension of the Heisenberg model — but unphysical.
- Model was solved by Theodore Berlin:
  - No transition for $d = 1$
  - No transition for $d = 2$
  - $\exists$ transition for $d = 3$: $kT_{\mathrm{c}} = 0.989\hbar J$
  - $\exists$ transition for $d \geq 4$, behaviour independent of d (behaviour is mean field)

Summary of “magnet” models

Table 4.3: Critical exponents for some universality classes

	d	n	α	β	γ	δ	ν	η
Mean field	any	any	0	$1/2$	1	3	$1/2$	0
2d Ising	2	1	0	$1/8$	$7/4$	15	1	$1/4$
3d Ising	3	1	0.11	0.33	1.24	4.79	0.63	0.04
3d XY	3	2	-0.01	0.35	1.32	4.78	0.67	0.04
3d Heisenberg	3	3	-0.12	0.37	1.40	4.8	0.71	0.04
3d spherical	3	∞	-1	$1/2$	2	5	1	0