Emergence of Quantum Phases in Novel Materials

VII Edition ICMM-CSIC Postgraduate Course

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Macroscopic properties are governed by conservation laws and broken symmetries:

- The high temperature state is disordered, uncorrelated, uniform and isotropic: it has the full rotational and translational symmetry of free space.
- As T lowers, new phases condense, with lower symmetry (broken symmetry states).

Long range order is created by short range forces but the details of the microscopic interactions are not important and universal behaviours at the phase transitions are found.

Outline

- Classical phase transitions
  - Concepts with examples and definitions
  - Landau theory
  - Criticality and universal behaviour
  - Goldstone modes, Mermin Wagner theorem
  - Kosterlitz Thouless transition
- Quantum phase transitions
  - Quantum Ising model
  - Mapping to classical mechanics

Bibliography

- “The theory of critical phenomena”. J.J. Binney, N.J. Dowrick, A.J. Fisher and M.E.J. Newman.
- ”Principles of Condensed Matter Physics”. P.M. Chaikin and T.C. Lubensky
- “Introduction to many-body physics” P. Coleman
- “Lectures on Phase Transition and Renormalization Group”. N. Goldenfeld.
- ”Introduction to phase transitions and critical phenomena” H.E. Stanley.
- “Quantum Phase transitions”. S. Sachdev
- “Quantum Phase transitions” M. Votja, Rep. Prog. Phys. 66, 2069–2110 (2003)

Symmetry

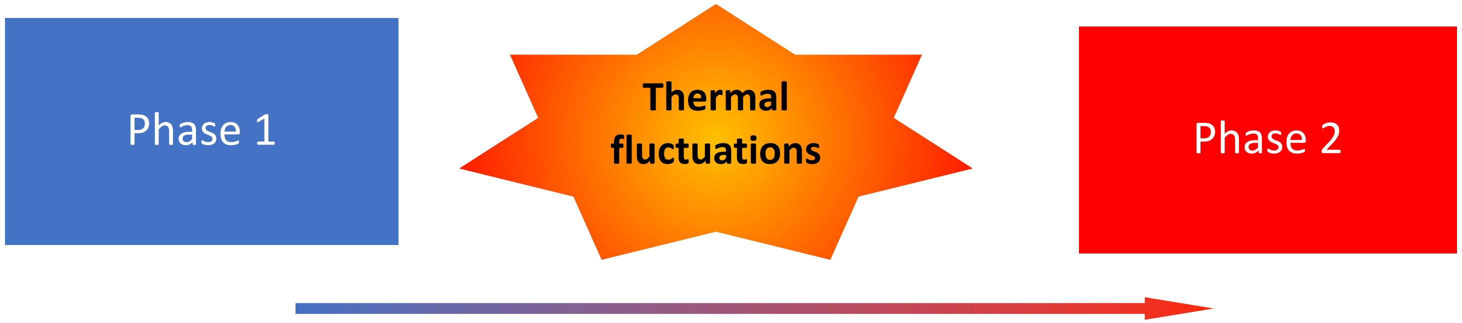
- The properties of any system of particles are determined by a Hamiltonian **H** which is invariant under some transformations (which form a group **G**).
- Possible transformations: translation, time reversal, rotation, reflection…
- Examples of groups:
  - Euclidian group: all spatial translations, rotations and reflections.
  - O(n): all rotations in an n-dimensional space.
  - U(1): isomorphic to O(2).
- Properties of groups:
  - Contain the identity
  - The combination of any pair of elements is also an element of the group.
  - Each element must have an inverse
- Symmetries can be continuous or discrete, global or local (gauge).

Classical versus quantum transitions

Thermal fluctuations versus quantum fluctuations

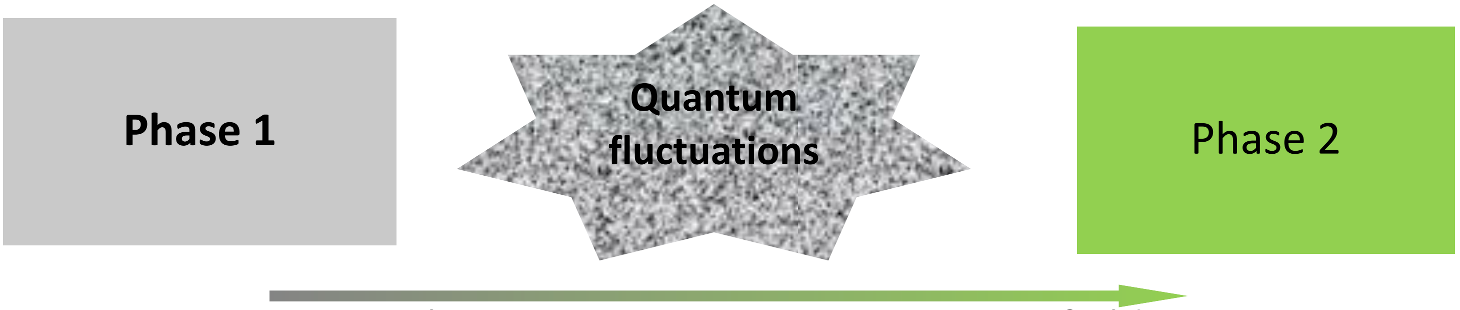
With temperature, even if the underlying phenomenon is quantum mechanical, the phase transition can be described classically.

Classical phase transition

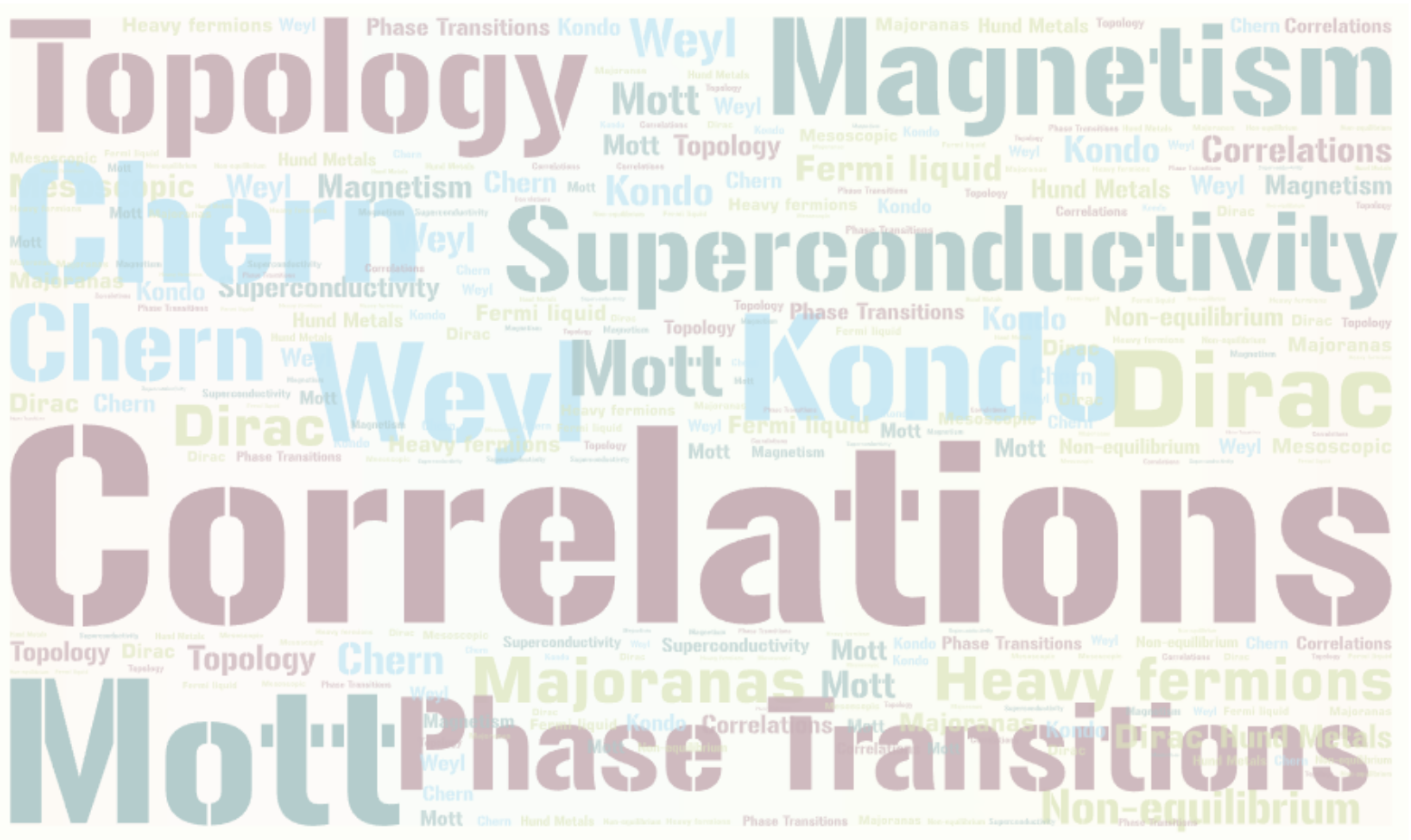


Control parameter: temperature…

Quantum phase transition
T=0, with effects on T>0



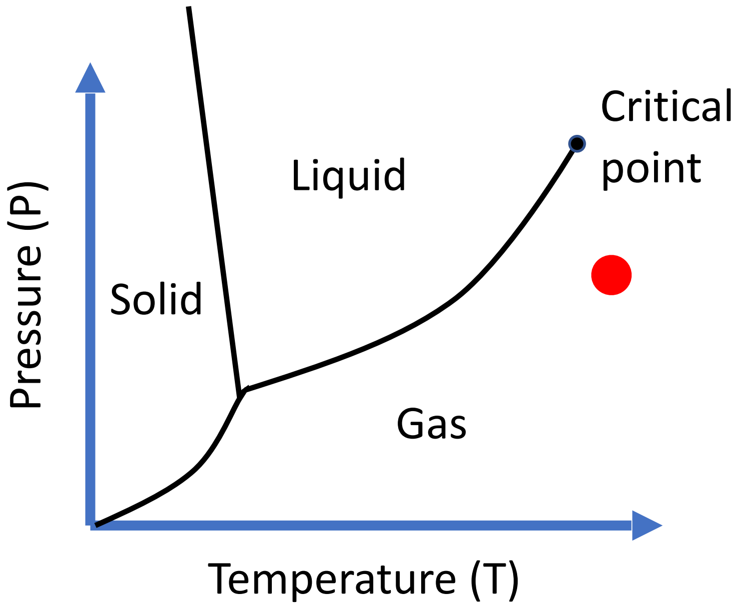
Control parameter: pressure, magnetic field, chemical composition…



Classical phase transitions

H_2O

PHASE DIAGRAM (sketch)



PD knobs

- Temperature
- Pressure

Critical point:

- Tc: 647 K, Pc: 2.2 x10^8 Pa

Triple point

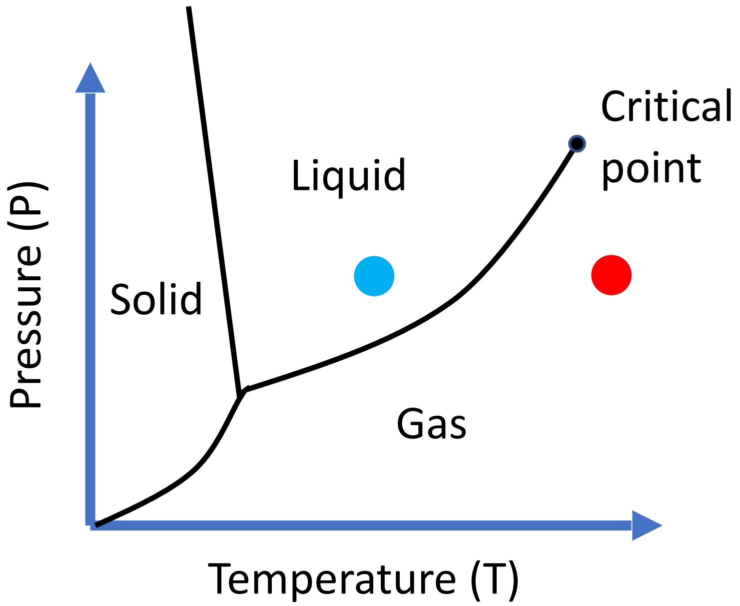
- T=0.01ºC, P=0.005 atm

High T:

- Kinetic energy dominates over potential energy due to intermolecular interactions → gas
- Full rotational and translational symmetry (density is uniform)

H_2O

PHASE DIAGRAM (sketch)



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- Full rotational and translational symmetry (density is uniform)

Lower T (lower kinetic energy)

- Attraction between molecules starts to dominate → density fluctuations → clustering
- Larger clusters have slower dynamics
- At a certain T, you get a liquid. Still full rotational and translational symmetry (density is uniform)

H_2O

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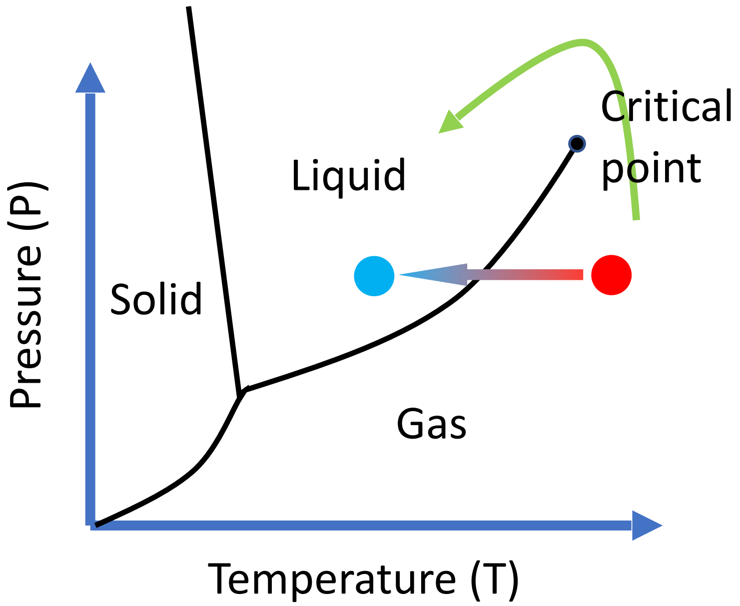
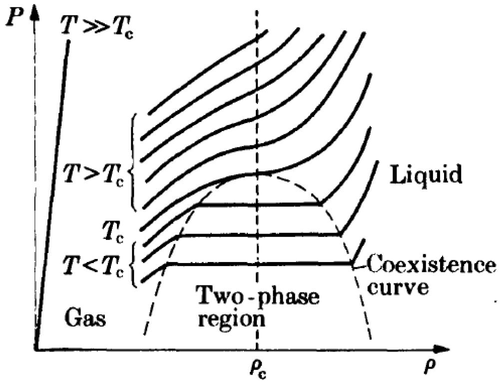


Isothermals:



- High T:
  - Kinetic energy dominates over potential energy due to intermolecular interactions → gas
  - Full rotational and translational symmetry (density is uniform)

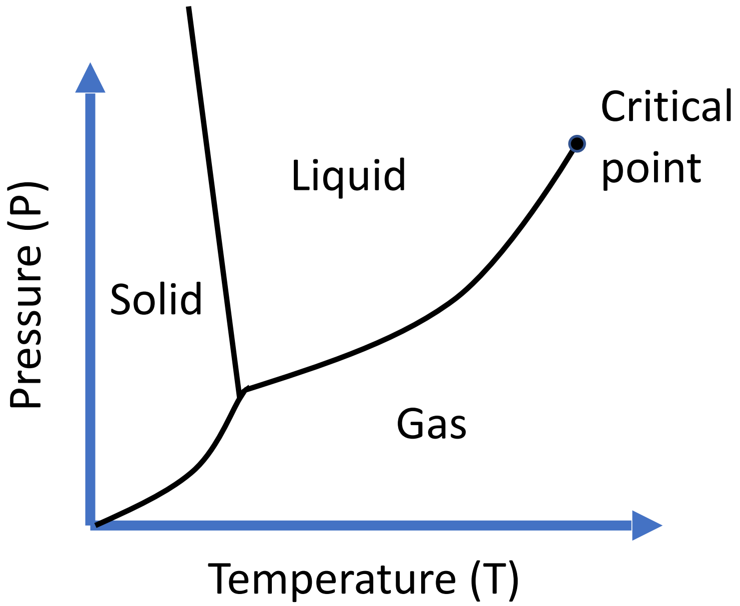
- Lower T (lower kinetic energy)
  - Attraction between molecules starts to dominate → density fluctuations → clustering
  - Larger clusters have slower dynamics
  - At a certain T, you get a liquid. Still full rotational and translational symmetry (density is uniform)

This is a **discontinuous** phase **transition**. At the line the two phases coexist. This phase transition requires energy (latent heat).

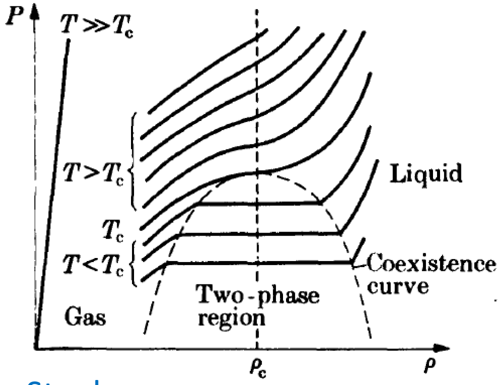
Liquid and gas have different densities and compressibilities but the same symmetry. By changing pressure and temperature, we could go from one to another without crossing a phase boundary!

H_2O

PHASE DIAGRAM (sketch)



Isothermals:



Stanley

Order parameter:

$\rho_L - \rho_g$

At the critical point (density ρ_c=0.322 g/cc, T_c=647 K, P_c=2.2 x 10^8 Pa), the transition is continuous (no phase coexistence)

At this continuous transition the compressibility (the capacity of a gas to change its density upon pressure) is very large (it diverges: a small change in pressure leads to a large change in density).

$$K_T = (\partial\rho/\partial P)_T$$

This divergence is associated to a divergent size of droplets and slowing down of fluctuations (critical behaviour). When the size of the droplets is of the order of the wave-length of visible light (0.5 μm) →critical opalescence.

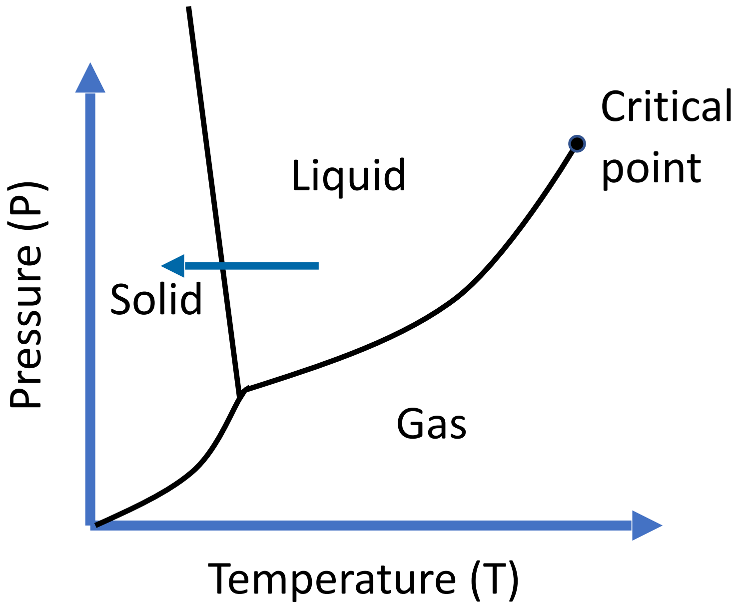
In general:

Continuous transitions are characterized by divergent **susceptibilities** (of which compressibility is an example).

Divergences occur following scaling laws: **critical exponents.**

H_2O

PHASE DIAGRAM (sketch)



PD knobs

- Temperature
- Pressure

Critical point:

- Tc: 647 K, Pc: 2.2 $\times 10^8$ Pa

Triple point

- T=0.01ºC, P=0.005 atm

Liquids are correlated: knowing the position of a molecule you can know the position of nearby molecules (within a distance called the **correlation length** ξ).

In a crystalline solid, the position of one molecule or atom determines the position of all the other ones in the system (long range order).

We distinguish liquids and solids for their symmetry:

- A liquid is isotropic and homogeneous (it is invariant under any continuous translation or rotation)
- A solid have ordered particles (only particular rotations and translations leave the system invariant).

The symmetry of the solid is lower than in the liquid.
The liquid-solid transition **breaks the continuous symmetry** of the liquid state. The system acquires **rigidity.**

The transition is characterised by an **order parameter,** the Fourier transform of the density: 0 in the liquid, finite in the solid).

MAGNETIC CONTINUOUS TRANSITIONS

Consider a set of magnetic dipoles (spin S) positioned in, for instance, a square lattice. S is the degree of freedom.

They interact through a quantum quantity called exchange J.

J is the coupling constant. It can be positive or negative.

Some typical models:

- Heisenberg model: continuous symmetry

(S can point on any direction)

$$H = -J\sum_{\langle i,j\rangle} \vec{S}_i \vec{S}_j$$

- Ising model: discrete symmetry

(possible values of σ are up and down)

$$H = -J\sum_{\langle i,j\rangle} \vec{\sigma}_i \vec{\sigma}_j$$

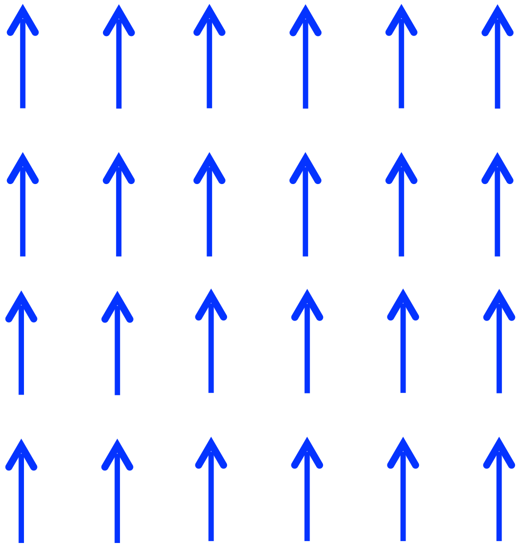
i and *j* are nearest neighbours

HEISENBERG MODEL

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j \qquad \text{(with } J>0\text{)}$$

Continuous symmetry case: O(3)

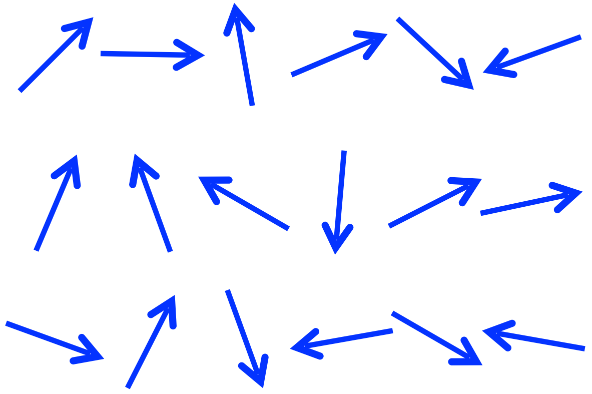
Low T: lower symmetry. Ferromagnet (FM)
Rotational symmetry is lost.



At T_c :
Spontaneous symmetry breaking

Diverging temperature fluctuations

High T: high symmetry. Paramagnet (PM): in time, any spin points in all directions with equal frequency. Continuous rotational symmetry.



Spins rotating in 3 spatial directions

Note: The hamiltonian is always invariant under rotational symmetry but the ground state (T<Tc) is not.
The low T phase could point in any of the directions in space!
One of the directions is "chosen" → spontaneous symmetry breaking.

HEISENBERG MODEL

$$H = -J\sum_{\langle i,j\rangle}\vec{S}_i\vec{S}_j$$

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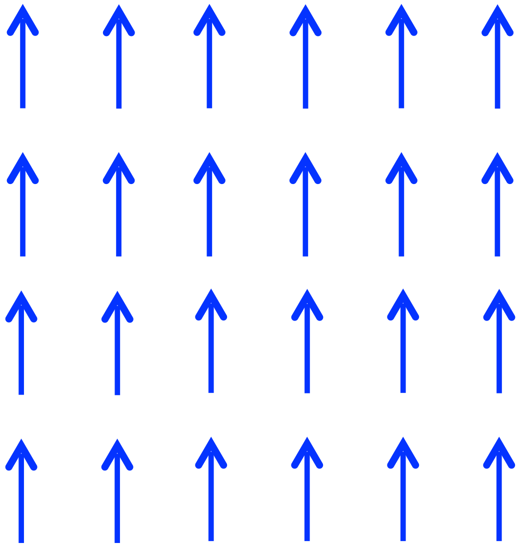

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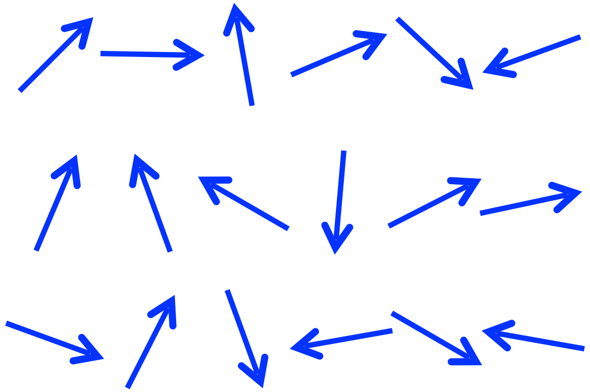


Spins rotating in 3 spatial directions

Correlation length ξ:

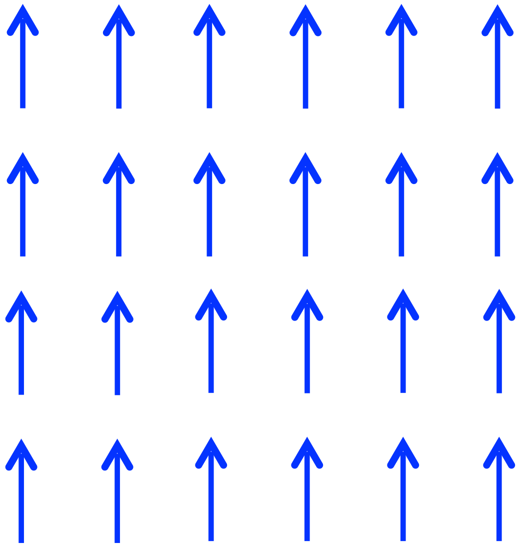
- related to the size of FM clusters that arise spontaneously at high T.
- FM clusters get larger as T decreases until it diverges at Tc (for the thermodynamic limit. For finite systems there cannot be a divergence → finite size effects).

HEISENBERG MODEL

$$H = -J\sum_{\langle i,j\rangle} \vec{S}_i \vec{S}_j$$

Continuous symmetry case: O(3)

FM: M≠0

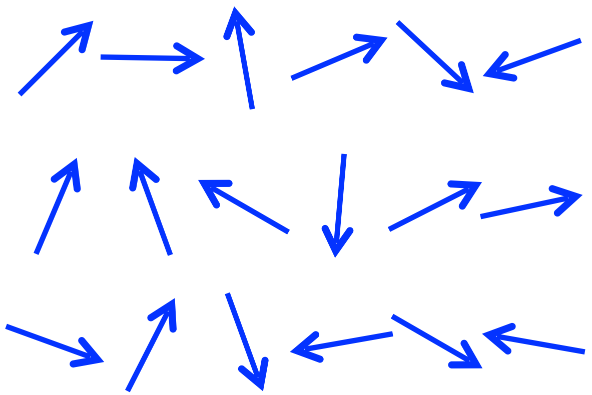


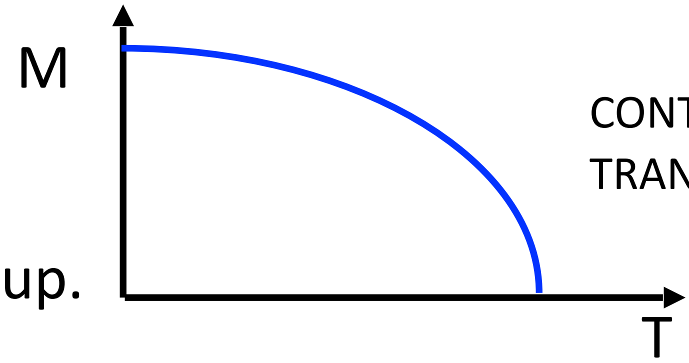
At T_c :

Spontaneous symmetry breaking

Diverging temperature fluctuations

PM: M=0





CONTINUOUS TRANSITION

Order parameter: magnetization $M = \langle \vec{S}_i \rangle$

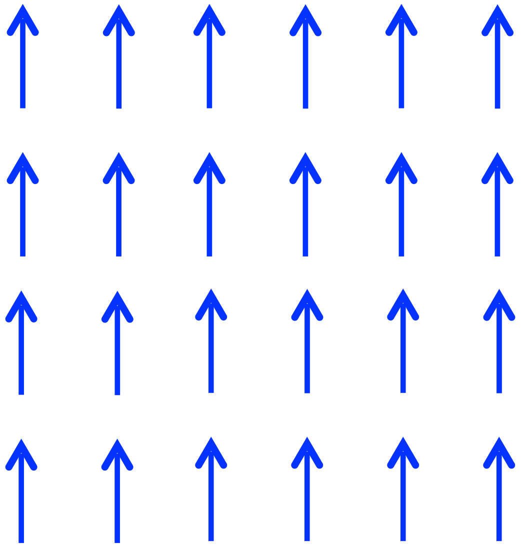
Note: The order parameter is not invariant under the O(3) group.

ISING MODEL

$$H = -J \sum_{\langle i,j \rangle} \vec{\sigma}_i \vec{\sigma}_j \qquad \text{(with } J>0\text{)}$$

Discrete symmetry case: Z_2

FM: M≠0



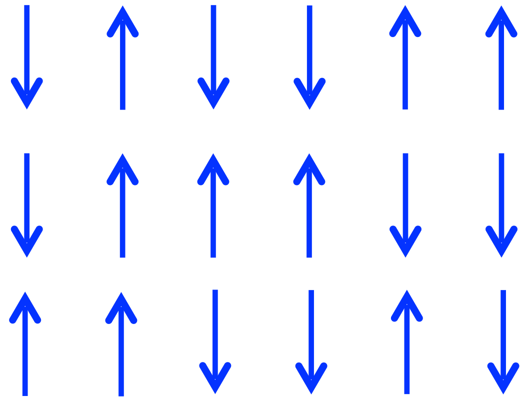
At T_c :

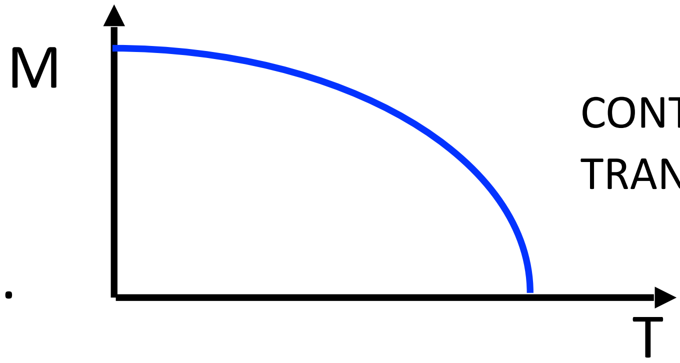
Spontaneous symmetry breaking

Diverging temperature fluctuations

PM: in time, any spin points in the two possible directions with equal frequency.

PM: M=0





CONTINUOUS TRANSITION

Order parameter: magnetization $M = \langle \vec{\sigma}_i \rangle$

Note: The order parameter is not invariant under the Z_2 group.

Spontaneous symmetry breaking

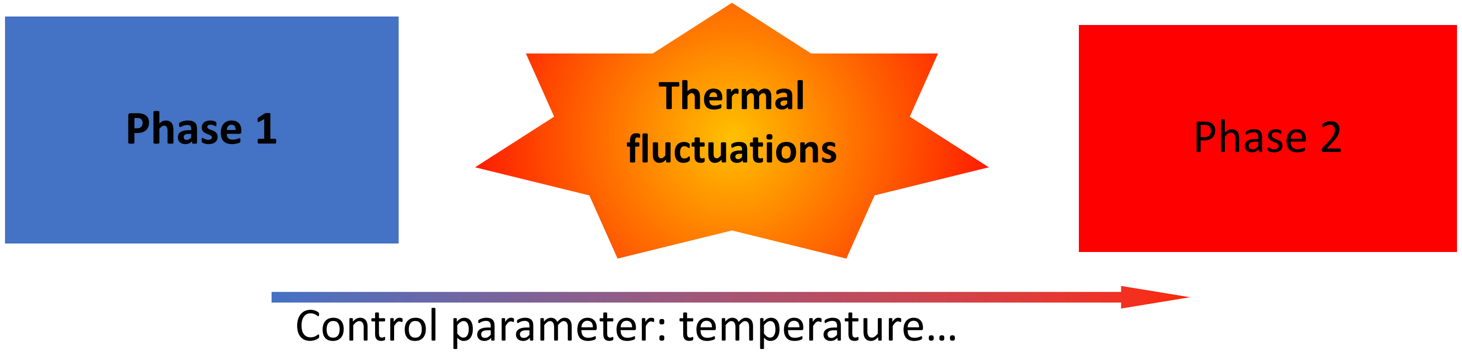
There are many possible symmetry broken states (i.e. all possible orientations of the magnetisation allowed by the symmetry of the Hamiltonian).

We can induce an order parameter by cooling in the presence of an external field h (conjugate field) that couples to the order parameter.
The conjugate field of the magnetisation is the external magnetic field:

$$H = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^z$$

For a finite system, thermal fluctuations generate domains and the order parameter averages to 0. The order parameter will be thermally stable in the thermodynamic limit.

$$\lim_{h \to 0} \lim_{N \to \infty} \langle \hat{\sigma}_i^z \rangle \neq 0$$



- All macroscopic properties can be deduced from the **free energy** (thermodynamic limit).

$$F = \langle H \rangle - TS$$

- At high T, *F* is dominated by entropy S: uncorrelated, isotropic, homogeneous, high symmetry.
- At low T: *F* is dominated by the interactions.
- At T_c: singularities of the free energy.

SUMMARY OF CONCEPTS (SO FAR)

- At high T
  - kinetic energy dominates over potential energy
  - high symmetry, higher entropy
- Lowering T, a transition may occur:
  - Continuous transition: divergence of characteristic lengths, susceptibilities and relaxation times. Continuous entropy. (Also called **second order phase transition**). **Critical phenomena**. **Universality.**
  - Discontinuous transitions: involves nucleation (or phase separation). Latent heat (jump in entropy). (Also called **first order phase transition**).
- Low T:
  - Potential energy dominates over kinetic energy
  - Lower symmetry phase (**spontaneous symmetry breaking**)
    - **Continuous** broken symmetry (as in liquid-to-solid water transition, Heisenberg model).
    - **Discrete** broken symmetry (Ising model)
- Phase transitions are characterized by order parameters (expectation value of a quantum operator)

Statistical mechanics

- A microstate is a possible microscopic configuration of the system (position and momenta, eigenstates…).
- The probability of finding the system in the microstate α with energy E_α is given, in thermal equilibrium, by the Boltzmann factor: $\exp(-E_\alpha/k_B T)$.
- Partition function $Z = \sum_\alpha e^{-\beta E_\alpha}$ with $\beta = (k_B T)^{-1}$.
- All properties can be calculated from Z. For instance, the average energy:

$$\langle E \rangle = \frac{1}{Z} \sum_\alpha E_\alpha e^{-\beta E_\alpha} = -\left(\frac{\partial \log Z}{\partial \beta}\right)_V$$

Also the free energy as $F = -\frac{1}{\beta}\log Z$

➢ Ex. Ising model in a magnetic field *h:* $$H = -J \sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^z$$

Order parameter: $M = -\frac{\partial F}{\partial h}$ $$\frac{\partial F}{\partial h} = -k_B T \frac{1}{\mathrm{Tr}\, \mathrm{e}^{-\beta \hat{\mathrm{H}}}} \mathrm{Tr} \frac{\hat{\sigma}_i}{k_B T} e^{-\beta \hat{H}} = -\langle \hat{\sigma}_i \rangle$$

Susceptibility: $$\chi = \frac{\partial M}{\partial h} = \frac{1}{\beta} \frac{\partial^2 lnZ}{\partial h^2}$$

Correlation functions: $$G^{(n)} \equiv \langle \sigma_1 \sigma_2 \ldots \sigma_n \rangle \propto \frac{1}{Z} \frac{\partial^n Z}{\partial h_1 \partial h_2 \ldots \partial h_n}$$

Connected correlation function: $$G_c^{(2)} \equiv \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$$

Give information about the fluctuations of the order parameter

Landau theory

- ➢Writes the free energy as a polynomial expansion of the order parameter M. (Valid for small values of the order parameter: close to a transition in a continuous phase transition).
- ➢Allowed terms only depend on the symmetries of the system.
- ➢It is a good description on length scales larger than the coherence length. It's a mean field theory. It doesn't know about the microscopic interactions.
- ➢For an Ising order parameter (Z_2 symmetry) only even power terms of M are allowed.

$$f = AM^2 + BM^4$$

Coleman

Landau theory for an Ising model

$$f = AM^2 + BM^4$$

with B>0

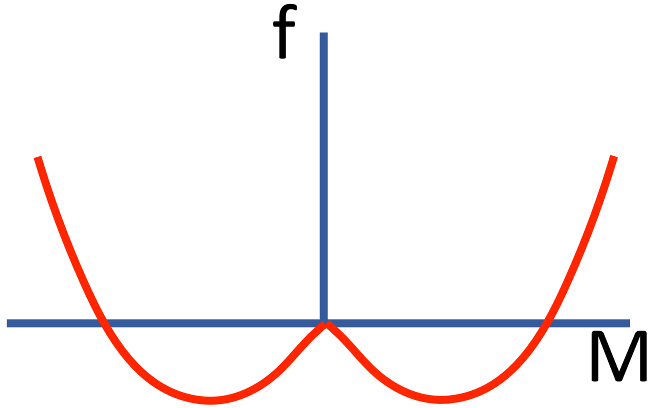
Calculate M as that which minimizes the Landau functional

$$\frac{\partial f}{\partial M} = 2AM + 4BM^3 = 0$$

A is chosen such that it changes sign at T_c

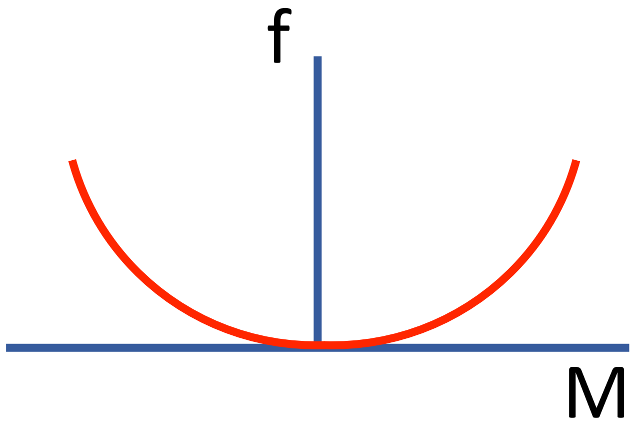
$$A = a(T - T_c)$$

A<0



$$M = \pm\sqrt{-A/2B}$$

A>0



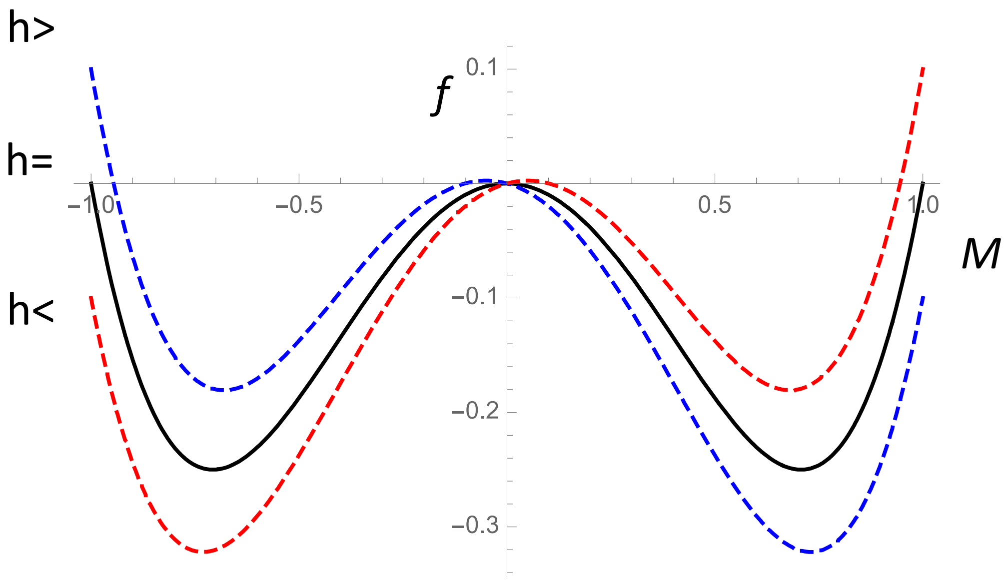
$$M = 0$$

$$M = \begin{cases} 0, & T > Tc \\ \pm\sqrt{\dfrac{a(T_c - T)}{2B}}, & T < T_c \end{cases}$$

With a magnetic field *h* $$f = AM^2 + BM^4 - hM$$

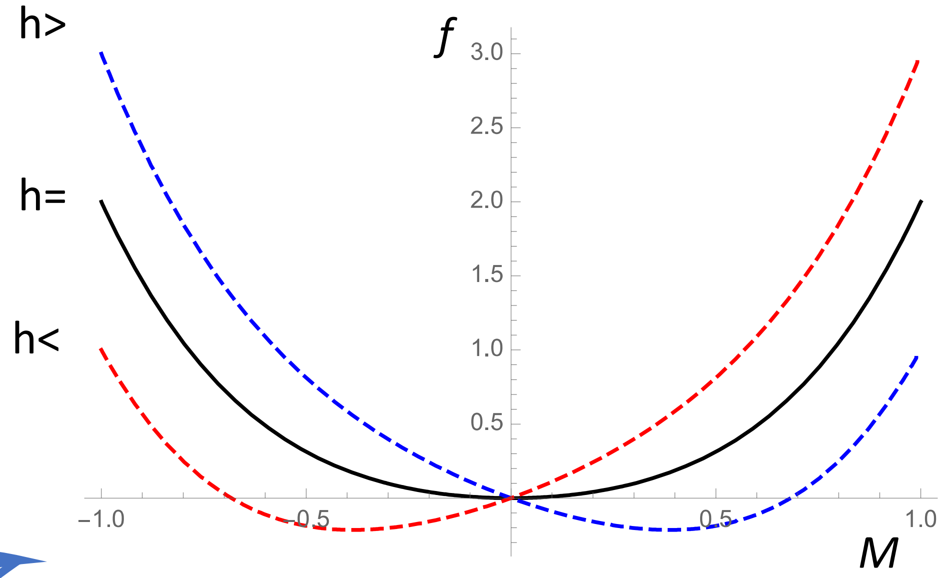
Discontinuous phase transition

$T<T_c$

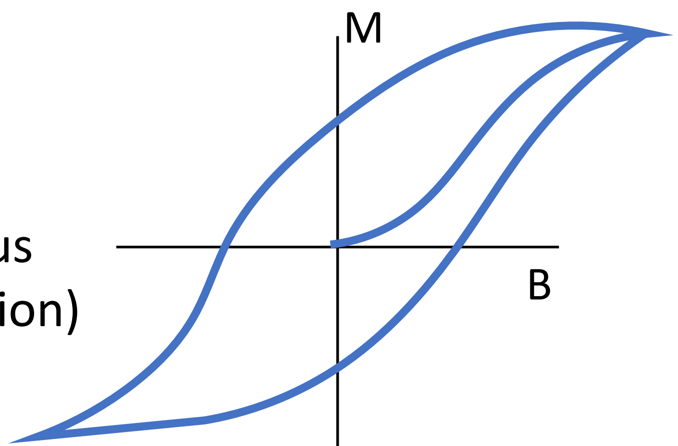


Continuous phase transition

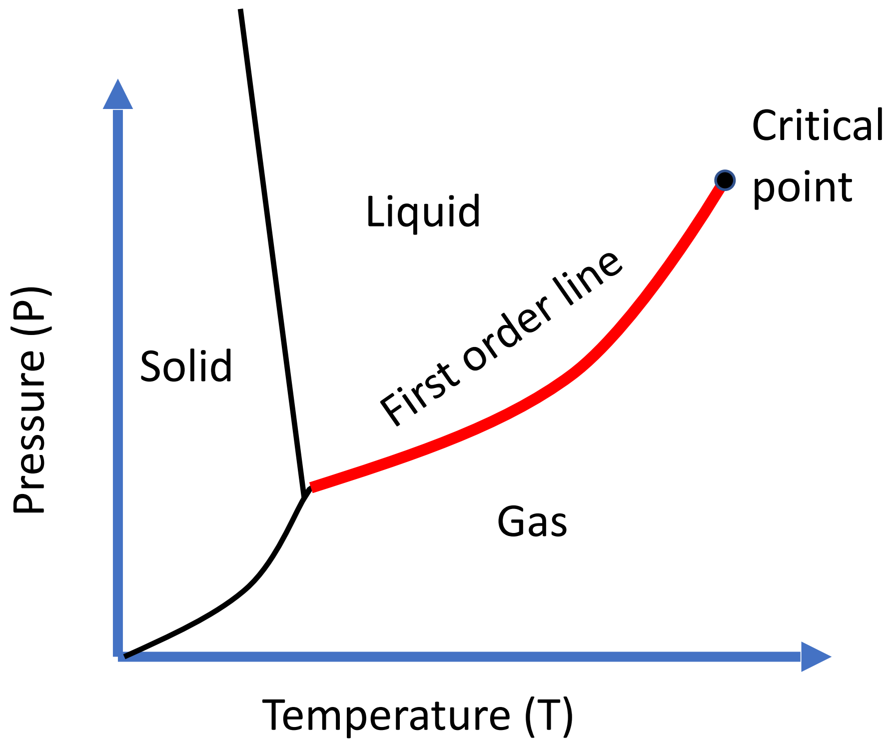
$T>T_c$

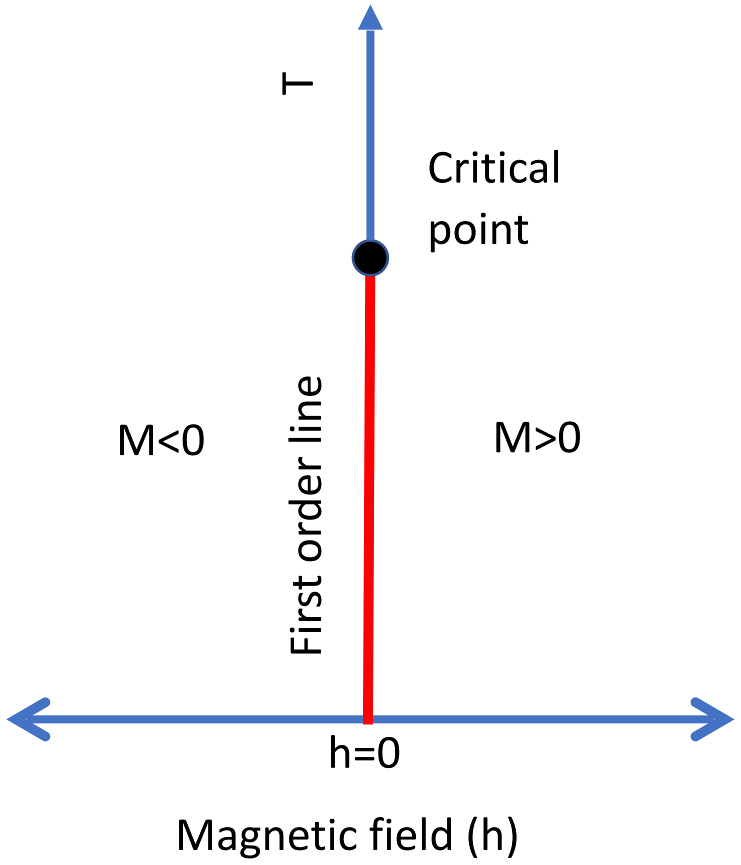


Hysteresis (discontinuous phase transition)



Note the analogy with the liquid gas transition: the magnetic field acts on the magnetization similarly to pressure on the gas and liquid densities.





At the transition T_c (with h=0):

$$f = AM^2 + BM^4$$

f is continuous

$$f = \begin{cases} 0 & (T > T_c) \\ -\dfrac{a^2}{4B}(T - T_c)^2 & (T < T_c) \end{cases}$$

The entropy S is continuous

$$S = \frac{\partial f}{\partial T} = \begin{cases} 0 & (T > T_c) \\ \dfrac{a^2(T_c - T)}{2B}, & T < T_c \end{cases}$$

The specific heat has a jump

$$C_V = -T\frac{\partial^2 f}{\partial T^2} = C_0(T) + \begin{cases} 0 & (T > T_c) \\ \dfrac{a^2 T}{2B} & (T < T_c) \end{cases}$$

The susceptibility diverges

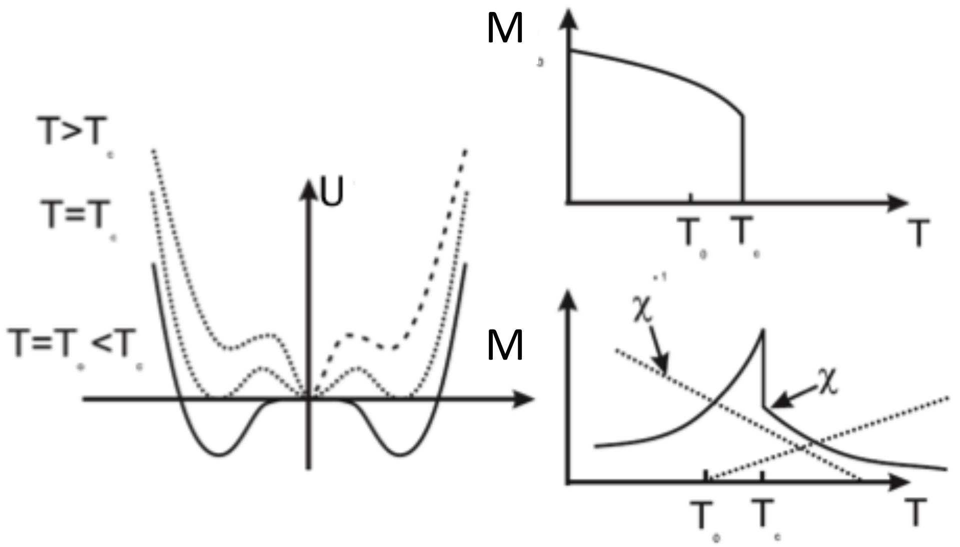
$$\chi = \frac{\partial m}{\partial h} = \frac{1}{a|T - T_c|} \times \begin{cases} 1 & (T > T_c) \\ \frac{1}{2} & (T < T_c) \end{cases}$$

Landau theory for discontinuous phase transitions

With B<0

(and go to next order in the order parameter expansion to get a finite M solution)

$$f = AM^2 + BM^4 + CM^6 - hM$$



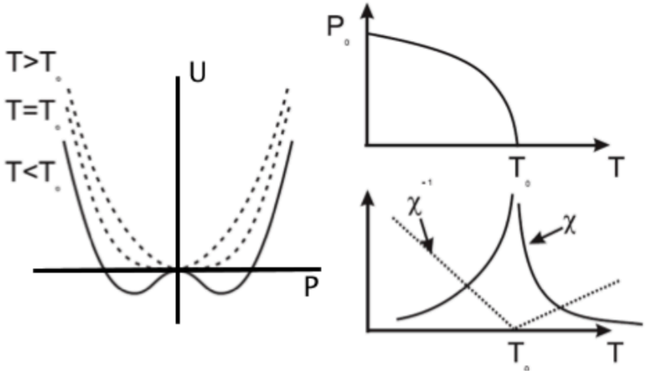
Both the order parameter and the susceptibility have a jump at T_c

Continuous vs discontinuous transitions

$$f = AM^2 + BM^4 + CM^6 - hM$$

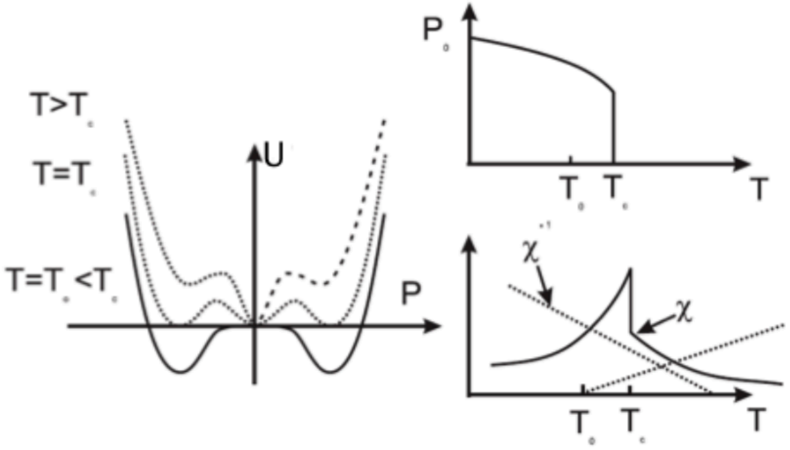
Continuous (2nd order) phase transition (B>0)

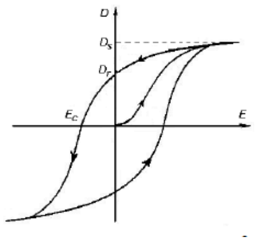
Continuous order parameter
Divergences at Tc: critical phenomena.



Discontinuous (1st order) phase transitions (B<0)

The order parameter and the susceptibility both have a jump at Tc.
There can be phase separation (negative compressibility). Hysteresis.





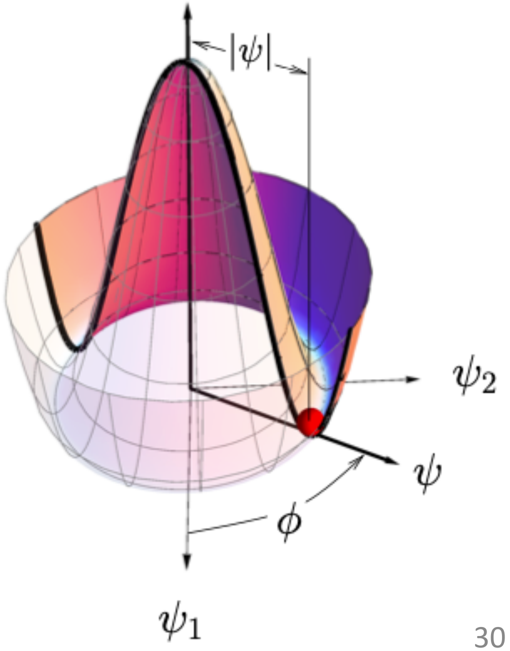
Landau for a continuous symmetry

Consider symmetry U(1) (isomorphic to O(2))

Order parameter is complex: $\Psi = \Psi_1 + i\Psi_2 = |\Psi|e^{i\phi}$

The free energy $f = A\Psi^*\Psi + B(\Psi^*\Psi)^2$ has a mexican hat shape:

The free energy is independent of the global phase ϕ.



When you break the continuous symmetry the system acquires a rigidity.
In order to include the rigidity we have to allow the order parameter to be inhomogeneous.

Coleman

Inhomogeneous order parameters: Ginzburg Landau

This theory was developed to study superfluidity (neutral fluid) and superconductivity (charged fluid).

Long-wavelength fluctuations can be added in Landau theory. $\phi(x)$ is slowly varying. The simplest functional (for a neutral fluid) is:

$$f_{GL}[T,\Phi] = \frac{c}{2}(\nabla\Phi)^2 + \frac{r}{2}\Phi^2 + g(T)\Phi^4 - h\Phi$$

Note $r = a(T - T_c)$

The correlation length ξ (characteristic length of the order-parameter fluctuations) can be introduced:

$$\xi(T) = \sqrt{\frac{c}{r}} = \xi_0 \left| 1 - \frac{T}{T_c} \right|^{-1/2}$$

With the coherence length:

$$\xi_0 = \xi(T=0) = \sqrt{\frac{c}{aT_c}}$$

ξ is the characteristic length for the correlation function $G_c^{(2)} \sim e^{-R/\xi}$ (close to Tc).

$$G(R) \propto |R|^{-d+2-\eta}$$

Scale invariance at T_c

Close to the critical point the correlation length is the only relevant length scale

⬇

we can rescale all lengths in the system by a common factor and at the same time adjust the external parameters in such a way that the correlation length retains its old value.

$$f(|T - T_c|/T, h) = b^{-d} f\left(\frac{|T - T_c|}{T} b^{1/\nu}, h b^{y_B} \right)$$

with b the scale factor

All observables depend on power laws → critical exponents

The singular behaviour close to the critical point is characterized by <u>critical exponents:</u>

Order parameter: $$\psi \propto \begin{cases} (T_c - T)^{\beta} \\ h^{1/\delta} \end{cases}$$

Correlation length: $$\xi \propto (T_c - T)^{-\nu}$$

Susceptibility: $$\chi \propto (T_c - T)^{-\gamma}$$

Specific heat: $$C \propto (T_c - T)^{-\alpha}$$

Two-point correlation function: $$G_c^{(2)}(r) \sim \frac{1}{r^{d-2+\eta}}$$ r large and T=Tc

Note that the Landau theory for an Ising model (or ϕ^4 theory) gives

β=1/2
ν=1/2
γ=1
α=0
$\delta = 3$

The exponents are related:
(only 2 are independent)

$$2 - \alpha = 2\beta + \gamma \qquad (2 - \eta)\nu = \gamma$$

$$2 - \alpha = \beta(\delta + 1) \qquad \nu d = 2 - \alpha$$

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The critical exponents depend on:
•Dimensionality of the space d
•Symmetries of the order parameter (dimensionality D)
but not on the details of the interaction (universality).

Table 1.2. Values of critical exponents

	Xe	Binary fluid	β-brass	^{4}He	Fe	Ni
D	1	1	1	2	3	3
α	< 0.2	$0.113 \pm .005$	$0.05 \pm .06$	$-0.014 \pm .016$	$-0.03 \pm .12$	$0.04 \pm .12$
β	$0.35 \pm .015$	$0.322 \pm .002$	$0.305 \pm .005$	$0.34 \pm .01$	$0.37 \pm .01$	$0.358 \pm .003$
γ	$1.3^{+.1}_{-.2}$	$1.239 \pm .002$	$1.25 \pm .02$	$1.33 \pm .03$	$1.33 \pm .015$	$1.33 \pm .02$
δ	$4.2^{+.6}_{-.3}$	$4.85 \pm .03$		$3.95 \pm .15$	$4.3 \pm .1$	$4.29 \pm .05$
η	$0.1 \pm .1$	$0.017 \pm .015$	$0.08 \pm .07$	$0.021 \pm .05$	$0.07 \pm .04$	$.041 \pm .01$
ν	≈ 0.57	$0.625 \pm .006$	$0.65 \pm .02$	$.672 \pm .001$	$0.69 \pm .02$	$0.64 \pm .1$

The theory of critical phenomena

Universality class:
same d and D.

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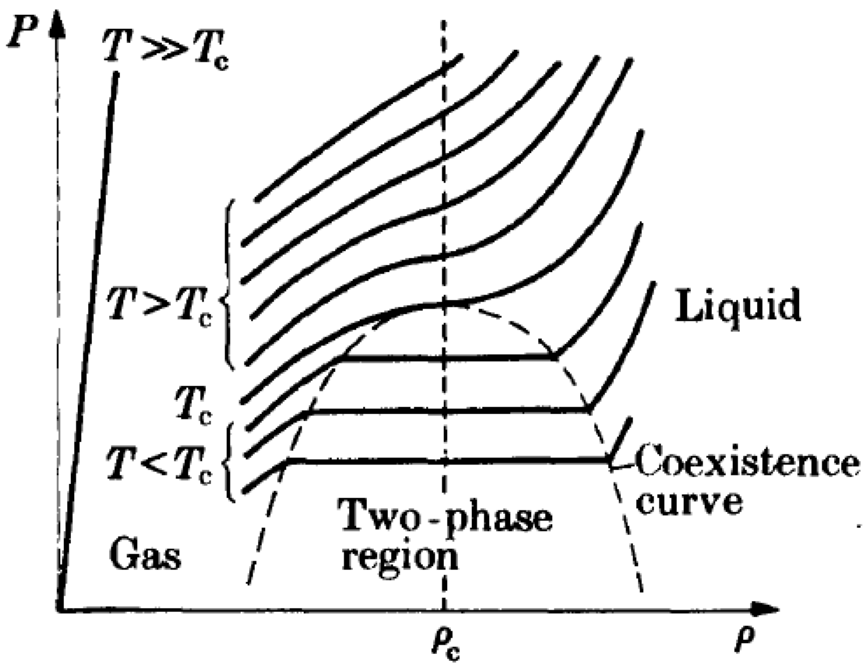
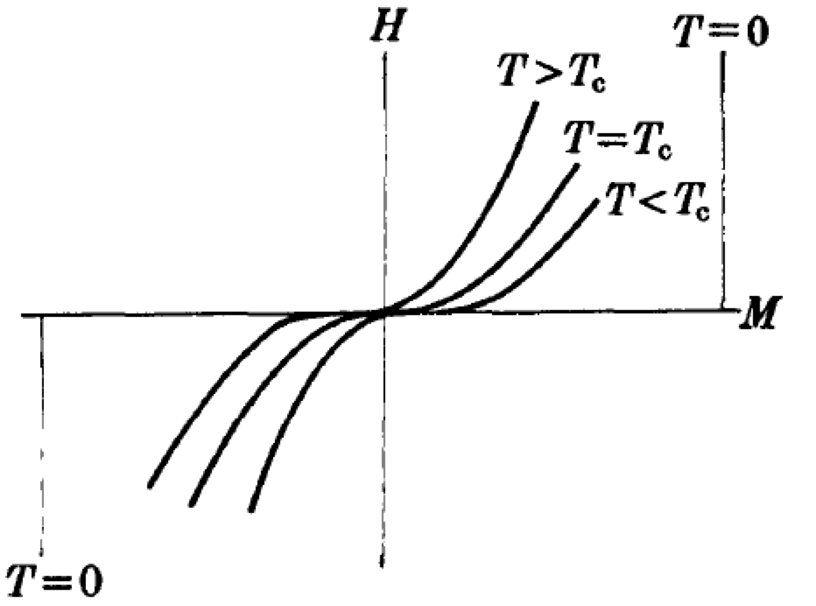
LIQUID-GAS



$$|\rho_L - \rho_g| \propto |T_c - T|^\beta$$

ISING FERROMAGNET



$$M \propto (T_c - T)^\beta$$

β ~0.32

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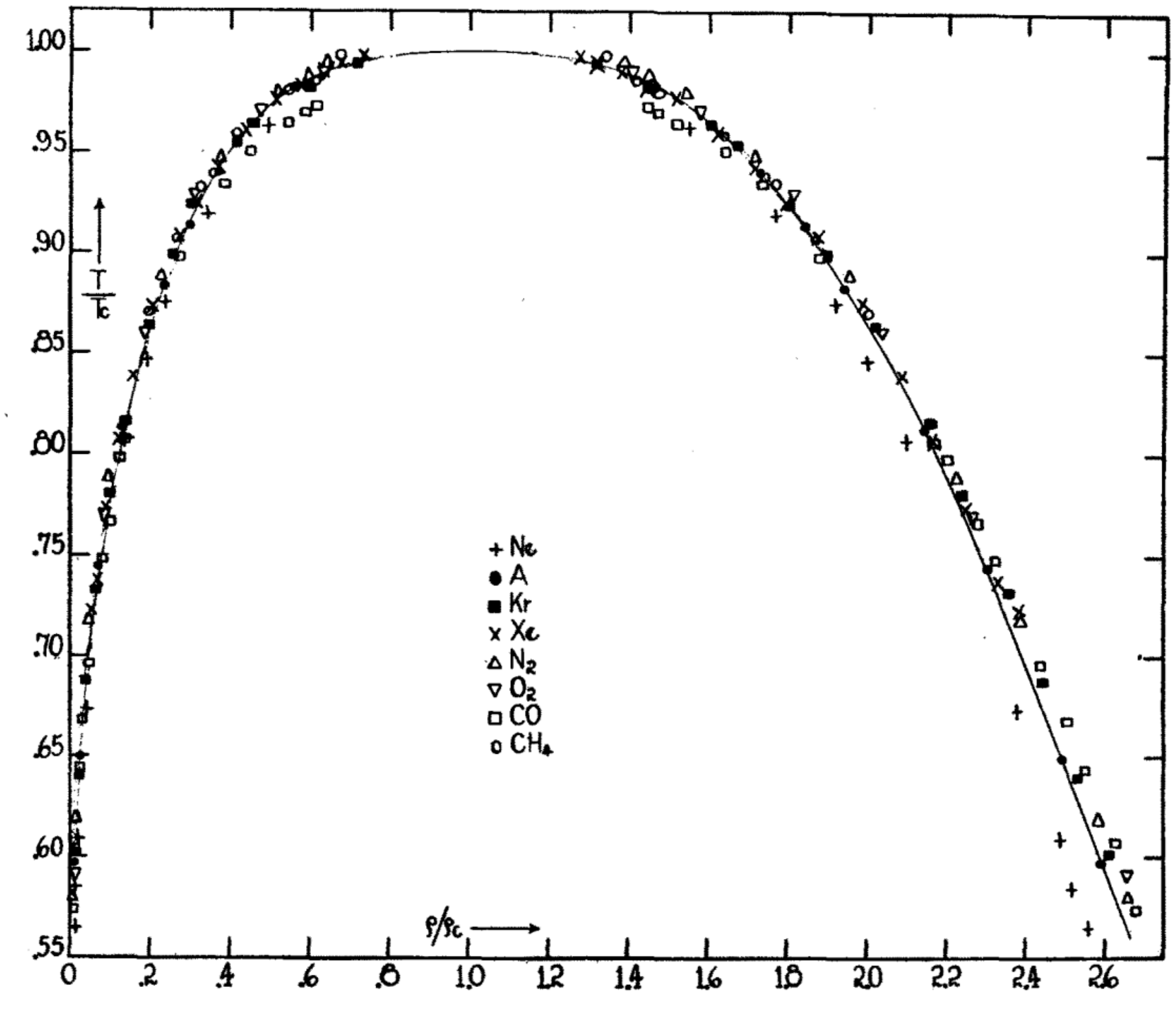


FIG. 2.

The liquid gas transitions of many fluids collapse into each other by scaling the variables: T/T_c and ρ/ρ_c (same for magnetic systems).

Guggenheim, The Journal of Chemical Physics 13, 253 (1945)

Validity of mean field

- ✓ The amplitude of the fluctuations has to be sufficiently small.
- ✓ Thermal fluctuations will tend to decrease Tc
- ✓ The amplitude of the fluctuations is small if the dimension of the system is larger than a critical dimension (d_c=4 for the Ising Universality class). This is stated by the Ginzburg criterion.
- ✓ If the coherence length is large, the deviation from mean field only affects very close to T_c. This is the case for conventional superconductors and superfluids.
- ✓ Beyond mean field →renormalization group (a procedure to eliminate high energy states keeping only what affects the low energy physics).

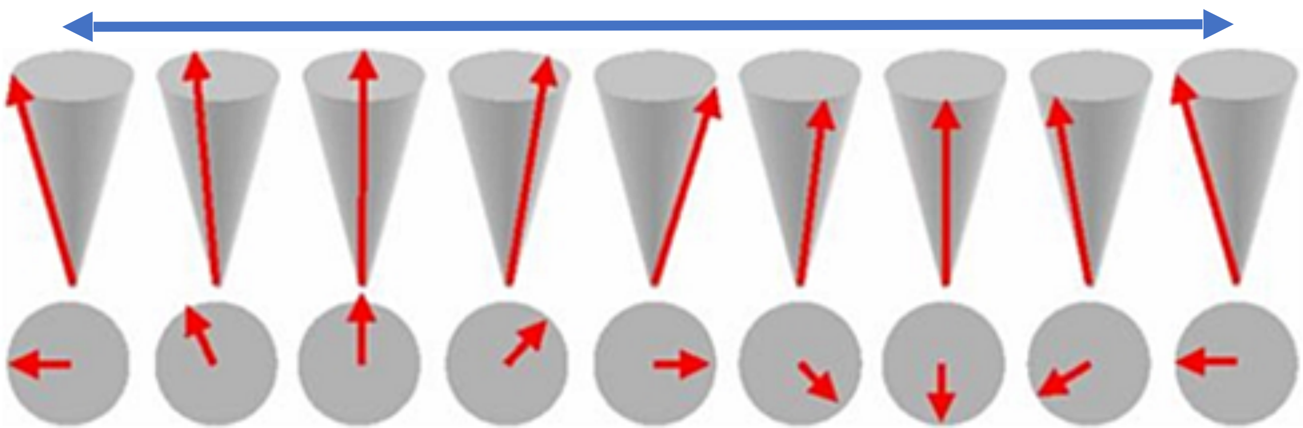
Goldstone modes and Mermin-Wagner theorem

Goldstone theorem

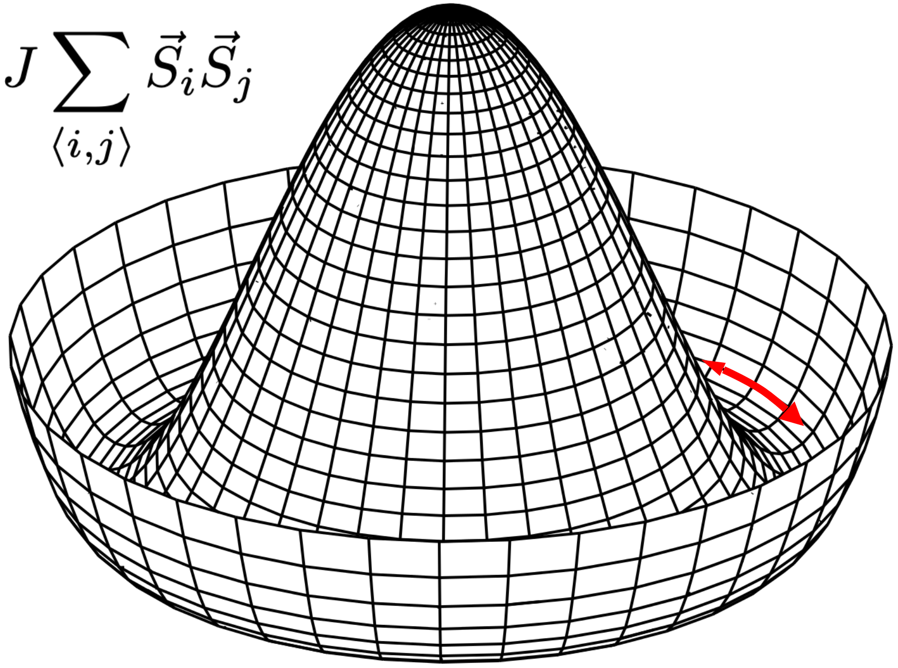
Low energy (long wavelength) excitations are possible in systems with continuous symmetry (namely, with a mexican hat potential).

Example: Heisenberg model [invariant under O(n)] $-J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j$

Spin-waves with wavelength λ.



Uni Münster



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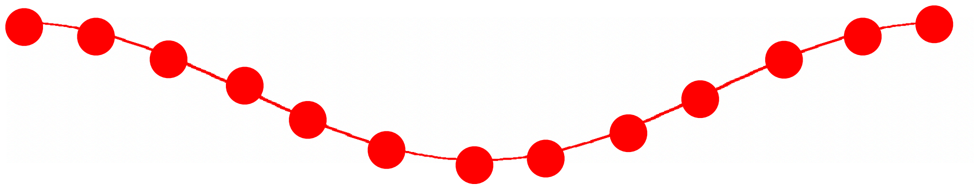
The cost of this excitation can be made vanishingly small: E ~q^2 (q →0 if λ→∞)

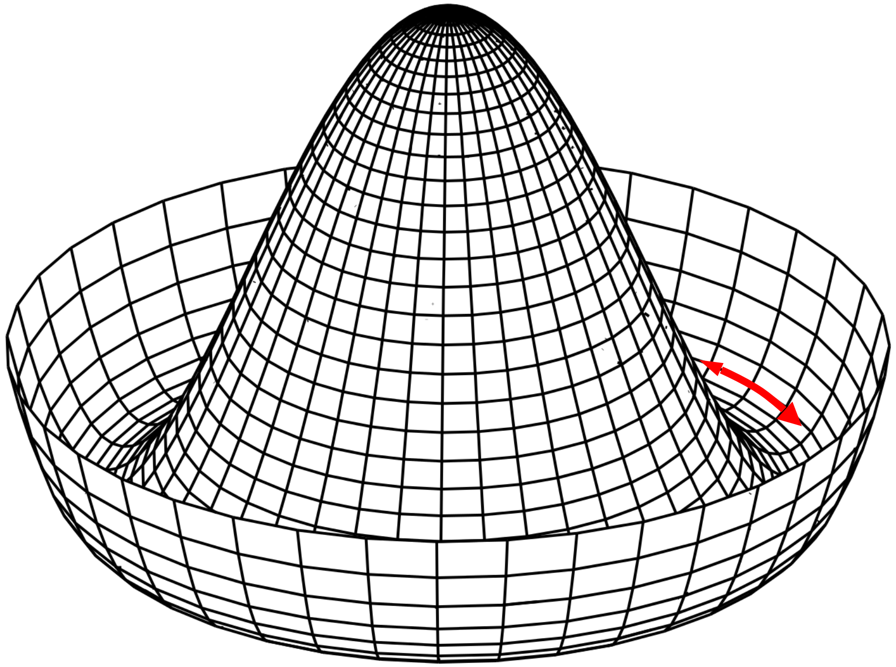
The excitations are massless Goldstone bosons. In the case of spins, these bosons are called **magnons**.

Goldstone theorem

Low energy (long wavelength) excitations are possible in systems with continuous symmetry (namely, with a mexican hat potential).

✓ In a crystalline solid: acoustic phonons
$E \sim |q|$.





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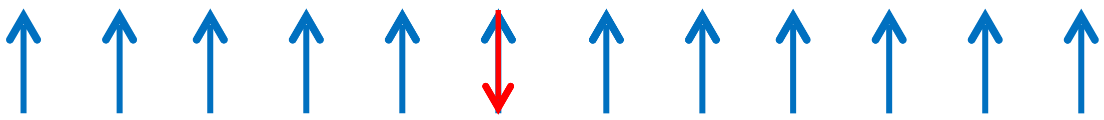
✓ In a superfluid (neutral fluid), Bogoliubov modes.

✓ BUT: a charged fluid (superconductor) develops a gapped spectrum: Anderson-Higgs mechanism.

If the symmetry is discreet:

Example: Ising model (Z_2 symmetry: up and down spins).

An excitation consists on flipping a single spin
(which involves a finite energy ~ J).



Therefore, a gapless excitation spectrum is not possible.

Mermin-Wagner theorem

Mermin, N. D. & Wagner, H. *Phys. Rev. Lett.* **17**, 1133–1136 (1966).

Goldstone modes gives rise to large fluctuation effects in low dimensions such that the ordered phase is destroyed.

In general, there is no phase transition for dimension $d \leq 2$ (for $T > 0$) if we have:

- Spontaneous symmetry of a continuous group (i.e not applicable to Ising model)
- Short range forces

The special case of d=2 and D=2: the Kosterlitz-Thouless transition

The XY model (D=2) in 2dim (d=2) has continuous symmetry U(1)/O(2), hence it cannot have a phase transition to a long-range ordered state (Mermin-Wagner).

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Berezinskii (1970), Kosterlitz and Thouless (1972) demostrated that the system undergoes a phase transition (though not long range ordered, there is not symmetry breaking).
The correlation function dies algebraically instead of exponentially (quasi-long range order).

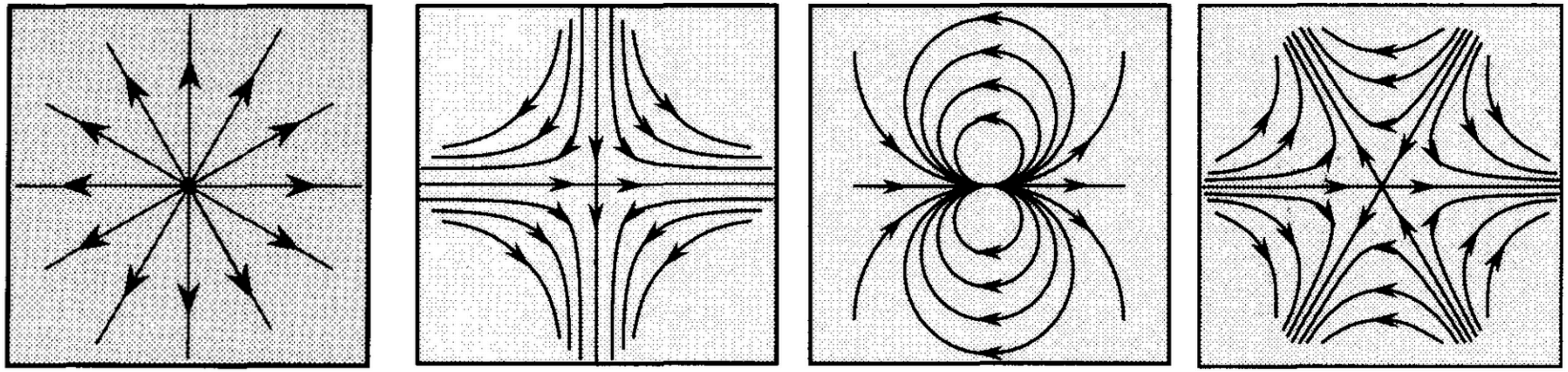
The special case of d=2 and D=2: the Kosterlitz-Thouless transition

The xy-model in 2dim has topological defects.

Vortices are characterized by the winding number n

$$\oint d\mathbf{r}\nabla\theta = 2\pi n$$

Chaikin & Lubensky



n=1 n=-1 n=2 n=-2

The special case of d=2 and D=2: the Kosterlitz-Thouless transition

Low T

Vortex-antivortex binding

Correlations show an algebraic decay $r^{-\frac{k_B T}{2\pi J}}$

(quasi long range order)

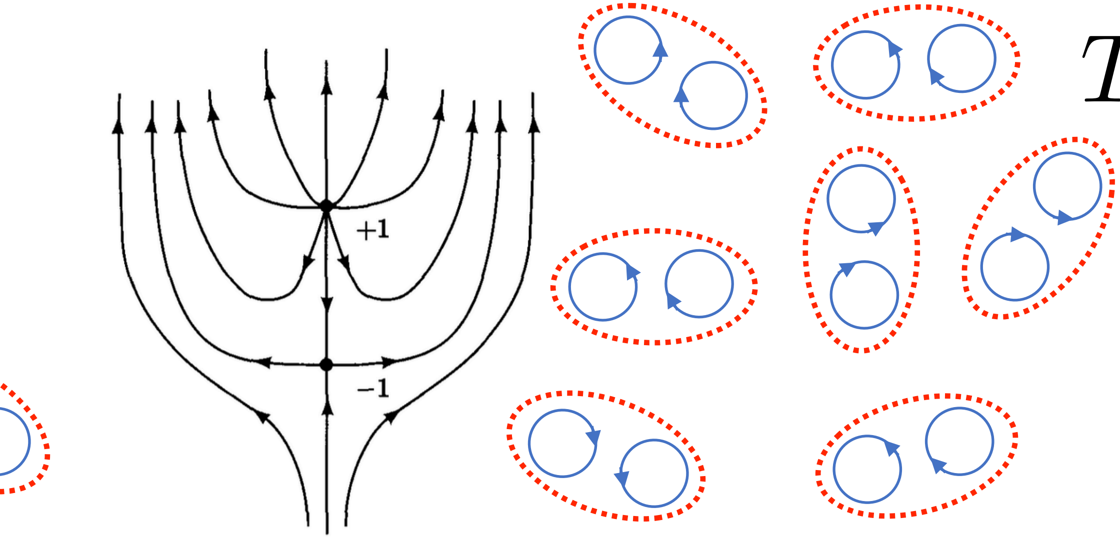
High T

Free vortices

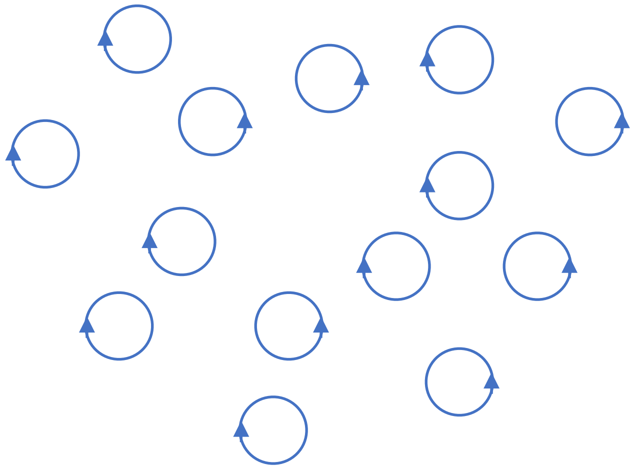
Exponential correlation decay $\exp\left(c/\sqrt{T-T_c}\right)$

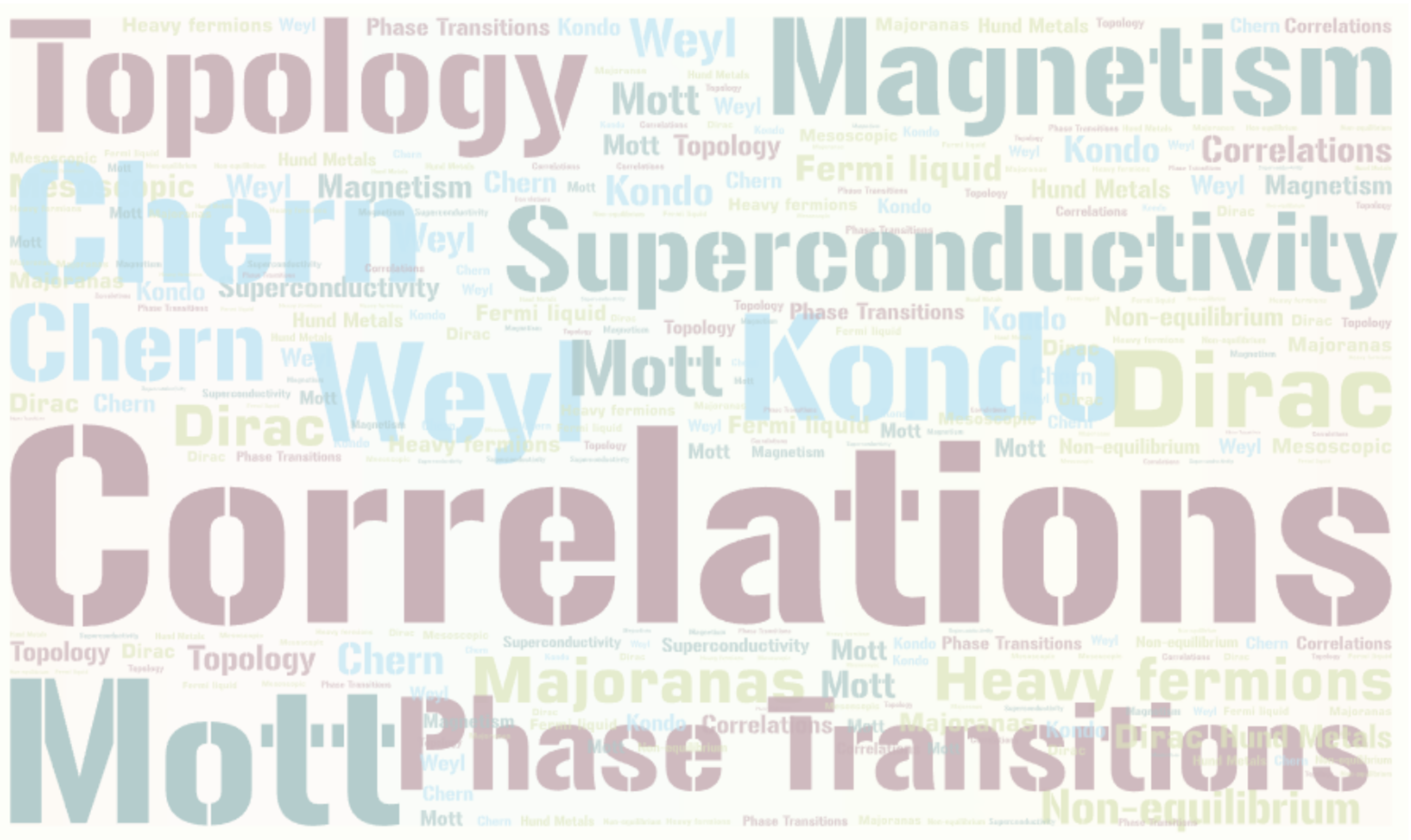
(disorder)

Pairs of vortices



$$T_{KT} = \frac{\pi J}{2k_B}$$

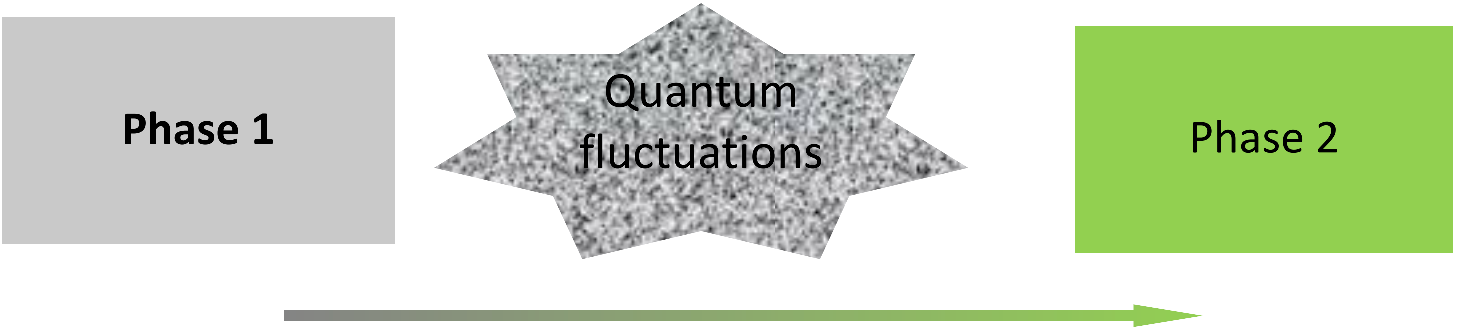




Quantum phase transitions

QUANTUM PHASE TRANSITIONS

Singularities in the ground state of the system (namely, at T=0).
Competing ground state phases.



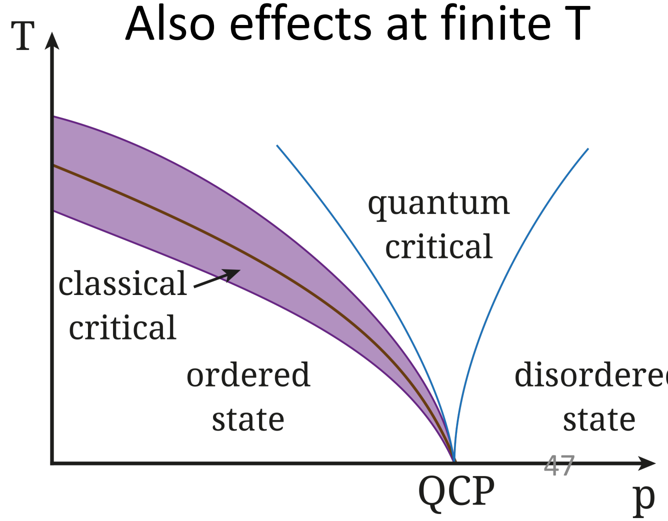
Control parameter: pressure, magnetic field…

Quantum fluctuations are driven by the Heisenberg uncertainty principle

$$H(g) = H_0 + gH_1$$

- Transition at g_c (a point of non-analyticity of the ground state).
- The nature of the correlations in the ground state changes qualitatively at g_c.

Also effects at finite T



Wikipedia

QUANTUM PHASE TRANSITIONS

$$H(g) = H_0 + gH_1$$

Transition at g_c

The characteristic energy scale of fluctuations is the gap
(Note: focusing on continuous phase transitions)

$$\Delta \propto |g - g_c|^{z\nu}$$

At g_c there is no gap →critical behaviour

The correlation length diverges

$$\xi^{-1} \propto |g - g_c|^{\nu}$$

The coherence time (time over which the wave function retains its phase) also diverges

$$\tau_\phi \propto \xi^z \propto |g - g_c|^{-\nu z}$$

z is the dynamic critical exponent

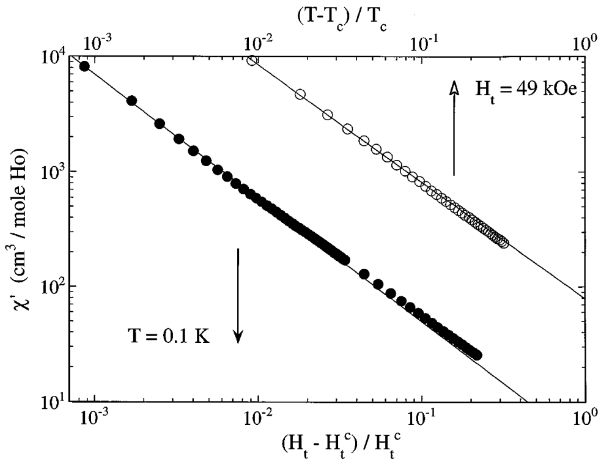
Quantum Ising model

$$H = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$

- ✓ g=0 is the classical Ising model. The ground state is a FM.
- ✓ Jg is a transverse (along x) magnetic field.

QPT observed in $LiHoF_4$ (FM with T_c=1.53K)

Phys. Rev. Lett. 77, 940 (1996)



Divergence of the susceptibility at T_c and at H_t^c

$$\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$ Eigenvalues σ_z=±1; eigenstates $|\uparrow\rangle, |\downarrow\rangle$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$ Eigenvalues σ_x=±1; eigenstates

$$|\rightarrow\rangle = (|\uparrow\rangle + |\downarrow\rangle)/\sqrt{2}$$

$$|\leftarrow\rangle = (|\uparrow\rangle - |\downarrow\rangle)/\sqrt{2}$$

GROUND STATE

For g<<1 (weak coupling) (classical solution)

$$|\uparrow\rangle = \prod_i |\uparrow\rangle_i \quad \text{or} \quad |\downarrow\rangle = \prod_i |\downarrow\rangle_i$$

In the thermodynamic limit:

$$\lim_{|x_i - x_j| \to \infty} \langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle = M^2$$

Long range order (spontaneous breaking of the Z_2 symmetry)

For g>>1 (strong coupling) the ground state is

$$|0\rangle = \prod_i |\rightarrow\rangle_i$$

And the values of σ_z are uncorrelated: $\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle = \delta_{ij}$

In general, for large g $\langle 0|\hat{\sigma}_i^z \hat{\sigma}_j^z|0\rangle \sim e^{-|x_i - x_j|/\xi}$

Quantum paramagnet

It is not possible to go from the g<<1 (magnetic order) to the g>>1 (quantum paramagnet) analytically →there must be a phase transition at some g_c

Exact spectrum for the Ising chain

$$H = -Jg\sum_i \hat{\sigma}_i^x - J\sum_{\langle ij\rangle} \hat{\sigma}_i^z\hat{\sigma}_j^z$$

It can be solved by applying a Jordan-Wigner transformation (it maps models with spin ½ to spinless fermions).

$$\epsilon_k = 2J(1+g^2-2g\cos k)^{1/2}$$

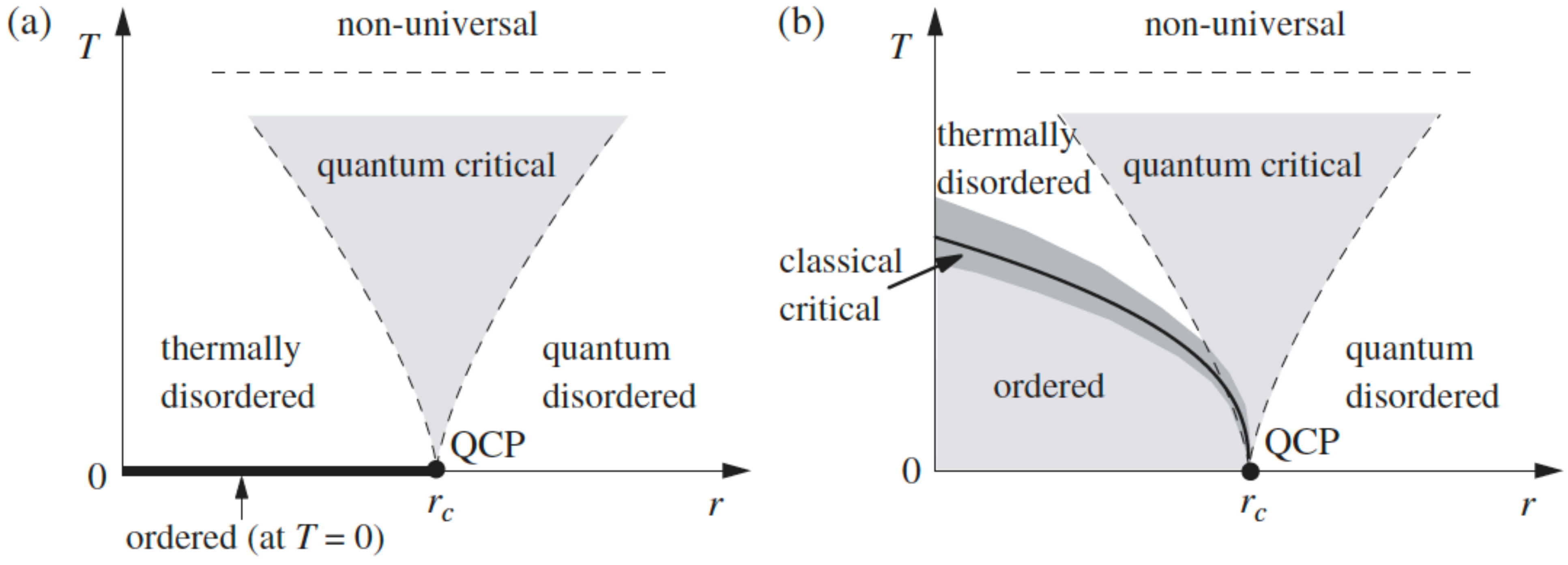
The mimimum excitation energy is at k=0 $\Delta = 2J|1-g|$ → g_c=1

$$\epsilon(k\to 0, g=1) \sim 2J(2-2(1-k^2/2))^{1/2} = 2J|k|$$

At g=1, fermions with low momenta must dominate.
This implies critical behavior.

Finite temperature phase diagram for the Ising chain

Quantum phase transitions also affect the finite T phase diagram



Low-T, outside of the quantum critical region: effective models of quasiclassical particles. Relaxation time is long.

In the quantum critical region, the relaxation time is short.

Mapping to classical mechanics

A quantum transition in d dimensions is connected to classical phase transitions in d+z dimensions. The additional dimension deals with (imaginary) time.

In a classical system with $H=H_{kin}+H_{pot}$, $[H_{kin},H_{pot}]=0$ → $Z=Z_{kin}\,Z_{pot}$
(statics and dynamics are decoupled and classical phase transitions can be studied using time independent theories)

In a quantum system the partition function doesn't factorize: statics and dynamics are coupled.

With $1/k_BT = \tau = -i\Theta/\hbar$

$$e^{-H/k_BT} \rightarrow e^{-H\tau}$$

Time evolution operator in imaginary time

Mapping to classical mechanics

A quantum transition in d dimensions is connected to classical phase transitions in d+z dimensions. The additional dimension deals with (imaginary) time.

In a classical system with $H=H_{kin}+H_{pot}$, $[H_{kin},H_{pot}]=0$ → $Z=Z_{kin}\,Z_{pot}$
(statics and dynamics are decoupled and classical phase transitions can be studied using time independent theories)

In a quantum system the partition function doesn't factorize: statics and dynamics are coupled.

New rescaling:

$$f(|g-g_c|/g,h) = b^{-(d+z)} f\left(\frac{|g-g_c|}{g} b^{1/\nu}, h b^{y_B}\right)$$

Compare to $$f(|T-T_c|/T,h) = b^{-d} f\left(\frac{|T-T_c|}{T} b^{1/\nu}, h b^{y_B}\right)$$

What is different about quantum transitions?

Although many properties can be calculated with this mapping, others need special attention:

✓ Some quantum models are qualitatively different from the classical counterparts, like some topological terms.

✓Calculating real time dynamics from imaginary time dynamics is tricky (it requires analytical continuation).

✓A new time scale arises, the phase coherence time τ_ϕ, with no analogue in the classical phase transitions.

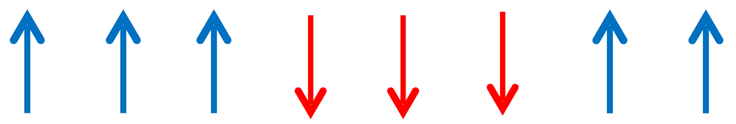
Outline

- Classical phase transitions
  - Concepts with examples
  - Landau theory
  - Criticality and universal behaviour
  - Goldstone modes, Mermin Wagner theorem
  - Kosterlitz Thouless transition
- Quantum phase transitions
  - Quantum Ising model
  - Mapping to classical mechanics

EXCITED STATES

For $g<g_c$

The excited states are domain walls (they cost energy)



$$\epsilon_k \sim J(2 - 2g\cos k + O(g^2))$$

For $g>g_c$

$$|i\rangle = |\leftarrow\rangle_i \prod_{j\neq i} |\rightarrow\rangle_j$$

$$\epsilon_k = Jg[2 - (2/g)\cos k + O(1/g^2)]$$