

Phase transitions in solid state and particle physics

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9h30-10h30

10h45-11h30

11h45-12h30

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1. Introduction

Literature:

J.M. Yeomans: Statistical mechanics of phase transitions
Oxford 1992, 144 S, ca. 60 €
readable and compact

P.M. Chaikin, T.C. Lubensky: Principles of condensed matter physics
Cambridge 1995, 684 S, ca. 50 €
concise, almost exclusively on phase transitions

I.D. Lawrie: A unified grand tour of theoretical physics
Bristol 1990, 371 S, ca. 50 €
really grand tour with many analogies

P. Davies: The New Physics
Cambridge 1989, 500 S, ca. 50 €
in-bed reading

other sources will be given 'on the ride'

Phase transitions in Heidelberg physics dep't.

- | | |
|---------------------------|-----------------------------------------------------|
| • Particle physics | Standard model ... |
| • Nuclear physics | Quark-gluon transition
Liquid-gas transition ... |
| • Atomic physics | Bose-Einstein
Laser |
| • Condensed matter | Glass transition
Surfaces
Biophysics ... |
| • Environmental physics | Condensation
Aggregation
Percolation ... |
| • Astrophysics, Cosmology | → next page |

History of the universe

Phase transitions of the vacuum:

Transition	Temperature	Time
Planck	10^{19} eV	~ 0 s
GUT's	?	?
Inflation	?	?
Electro-weak	100 GeV	10^{-12} s

Phase transitions of matter, i.e. freeze out of:

Quark-gluon plasma to nucleons	100 GeV?	10^{-12} s ?
Nucleons to nuclei	1 MeV	1 s
Atoms	10 eV	
	10^5 a	
Galaxies	3 K	today

Topics not treated

Phase transitions are a subfield of non-linear physics

Not treated are these 'critical phenomena':

- Route to chaos

- Turbulence

- Self organized criticality (forest fires, avalanches, ...)

- ...

Also not treated are these topics on phase transitions:

- Bose-Einstein condensates

- Superfluidity

- Quark-Gluon Plasma

- Quantum phase transitions

- Aggregates

- Fragmentation

- Percolation

- Liquid crystals

- Isolator-metal transitions

- Topological defects

- Traffic jams

- ...

2. Phenomenology

"Phenomenology of phase transitions"

derived from φαίνω = I appear, shine:

'phase' of moon as a periodic 'phenomenon',

'phase' = aggregate state as 'phenomenon',

'phantasy', 'fancy', ...

Four 'elements':

- earth = solid
- water = liquid
- air = gas
- fire = plasma

are the four aggregate states.

Control parameter

Phase transition = sudden change of the state of a system (probe)
upon a small change of an external parameter:
parameter reaches '**critical value**'.

more general: sudden shifts in behavior
arising from small changes in circumstances

In most of the cases treated in this lecture this control-parameter is temperature
(it can also be pressure, atomic composition,
connectivity, traffic density, public mood, taxation rate, ...):

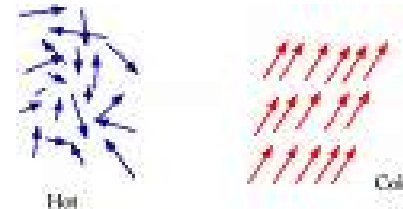
1st example: magnet

T_C = critical temperature:

below T_C : ferromagnet **FM**

above T_C : paramagnet **PM**

here: T_C = Curie temperature



The transition is an order-disorder transition: **PM**: disorder **FM**: order

Iron (Fe): $T_C(\text{Fe})=744^\circ\text{C}$ (dark red glow)

Order parameter

Below the critical temperature the probe suddenly acquires a property, described by a parameter M :

below T_C : $M \neq 0$,

which it did not have above the critical temperature:

above T_C : $M = 0$.

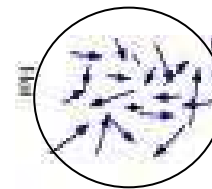
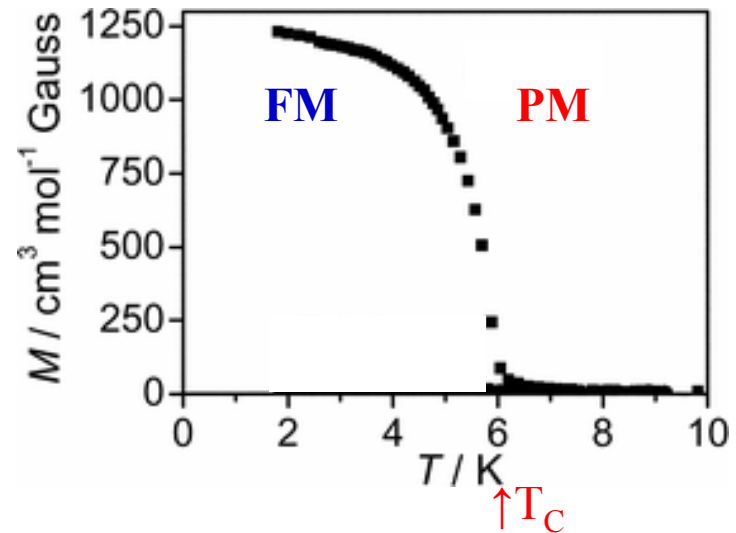
This parameter M is called the order-parameter:

Our example:

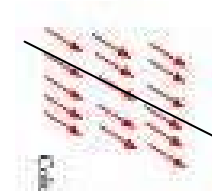
Order parameter = magnetisation M

(natura **facit** saltus)

N.B.:	Disorder:	high symmetry:
		↓
	Order:	low symmetry:



PM: rotational symmetry



FM: cylindrical symmetry

Critical exponent

Observation:

Near T_C the order M parameter depends on temperature T like:

above T_C : $M(T) = 0$ **PM**

below T_C : $M(T) = M_0 (1 - T/T_C)^\beta$ **FM**

with critical exponent β .

Examples:

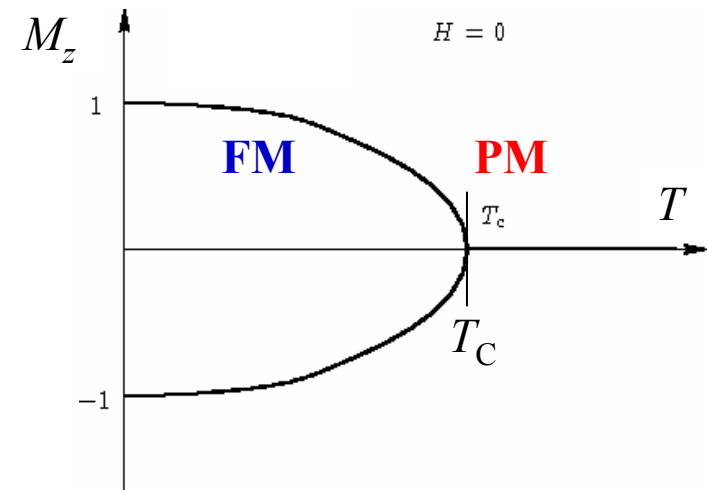
$$M(T) \sim \sqrt{(T_C - T)} :$$

critical exponent $\beta = 1/2$

$$M(T) \sim \sqrt[3]{(T_C - T)} :$$

critical exponent $\beta = 1/3$

1-dimensional magnet:
"bifurcation"



Comparison with experiment

With reduced temperature

$$t = (T_C - T)/T_C$$

and

$$m = M/M_0:$$

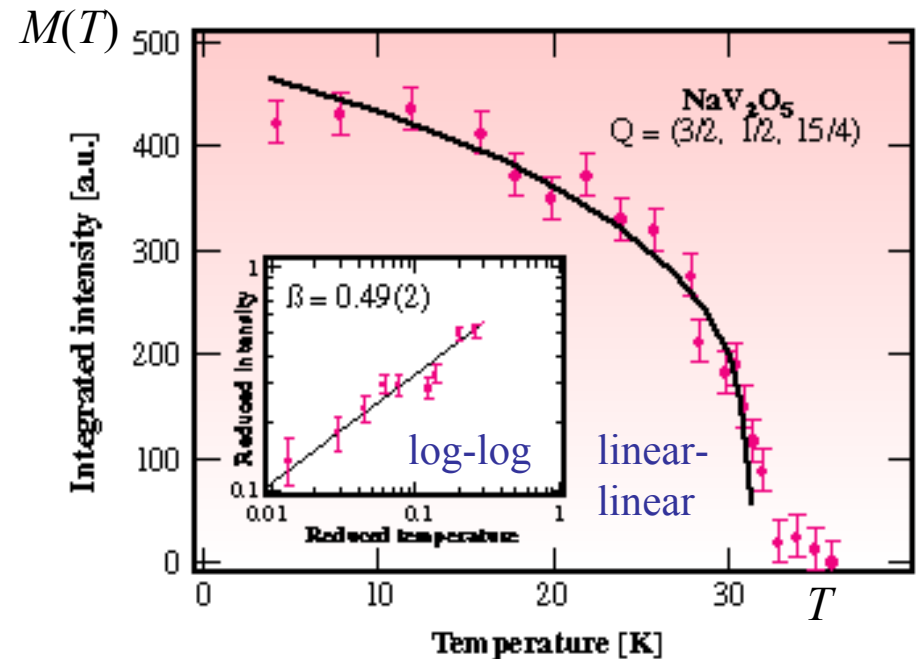
the order parameter scales with temperature

$$m = t^\beta,$$

as

or

$$\ln m = \beta \ln t$$



Temperature dependence of magnetisation measured by magnetic scattering of x-rays (European Synchrotron Radiation Facility) or of neutrons (Institut Laue Langevin)

Grenoble

ILL→
ESRF→



←Belle
donne

←Bastille

general view of Grenoble and the Polygone Scientifique

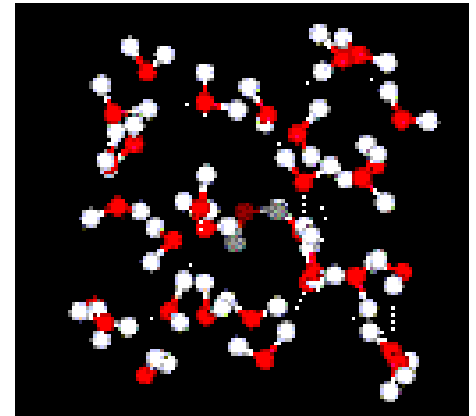
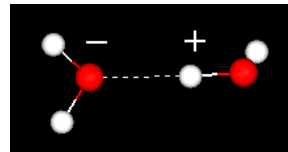
A 'run-away' phenomenon

Why are phase transitions so sudden?

2nd example: liquid

below T_C : liquid **L**

above T_C : gas **G**



Example of boiling water:

when a bond between 2 molecules breaks due to a thermal fluctuation, then there is an increased probability that a 2nd bond of the molecule with another neighbour breaks, too.

below T_C : broken bond heals, before 2nd bond breaks – water in boiler is noisy

above T_C : broken bond does **not** heal, before 2nd bond breaks – water boils:

A 'run-away' or 'critical' phenomenon: **L** \rightarrow **G**

Latent heat

Heat a block of ice:

Melting **S** \rightarrow **L**

Transition: order \rightarrow short range order

Boiling **L** \rightarrow **G**

Transition: short range order \rightarrow disorder

Breaking of bonds requires energy = latent heat
= difference in electrostatic molecular potential,

without change in temperature,
i.e. same kinetic energy of molecules.

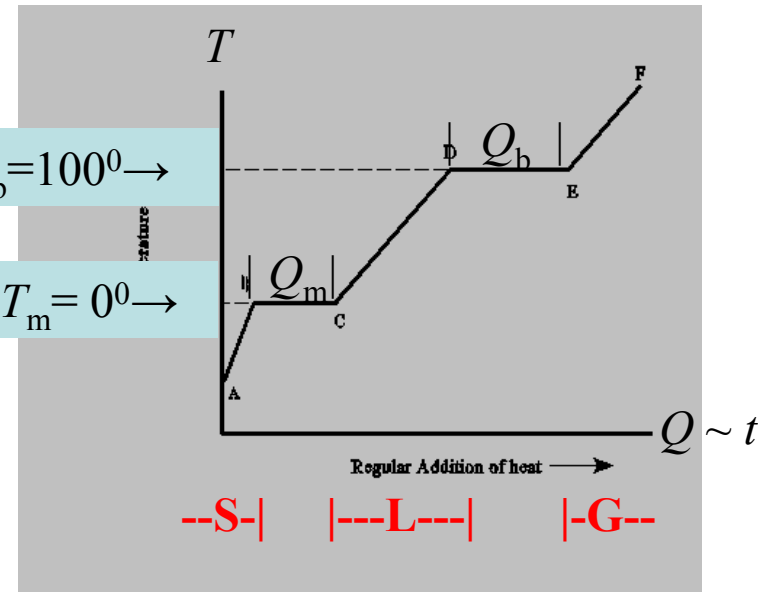
At critical temperature T_C :

Addition of heat only changes mass ratios
ice/water or water/vapor, but not the temperature

Water (H_2O):

boiling: $T_b = 100^\circ \rightarrow$

melting $T_m = 0^\circ \rightarrow$

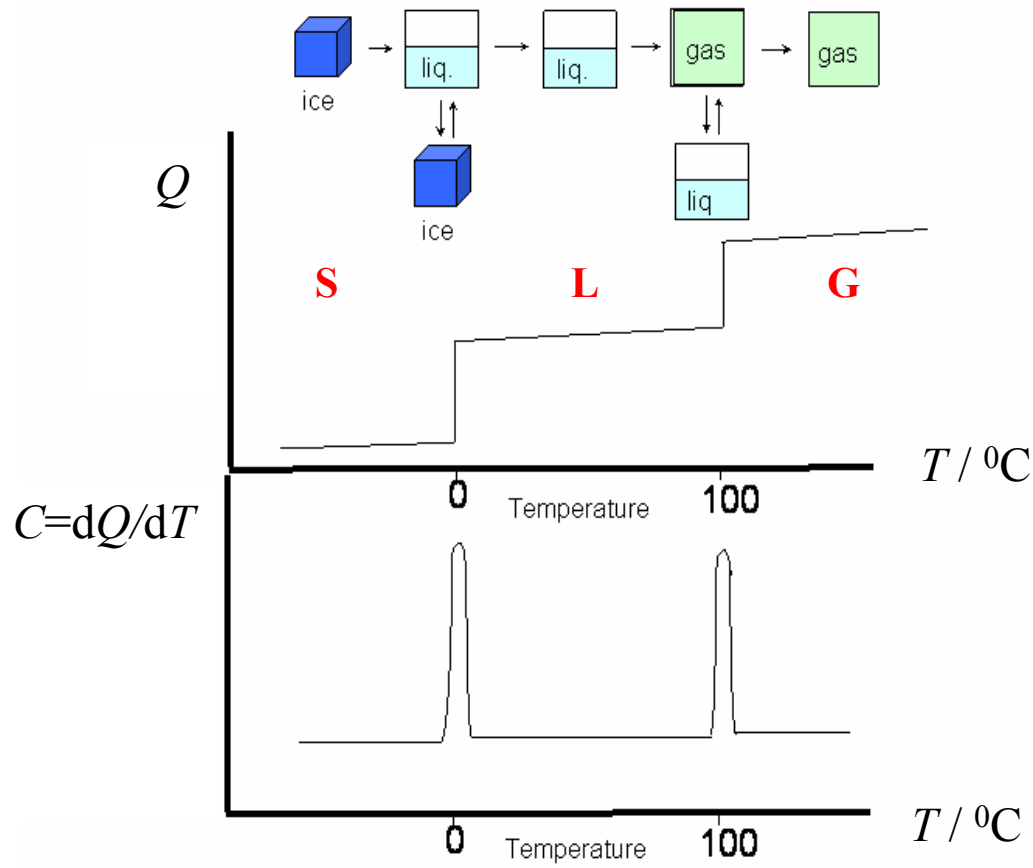


heat of melting $Q_m \uparrow$

heat of evaporation $Q_b \uparrow$

Divergence of heat capacity

When there is latent heat, the heat capacity dQ/dT diverges.



1st order vs. continuous phase transitions

Latent heat: $Q_b = \int_{L \rightarrow G} P dV = \text{area in } P\text{-}V \text{ diagr.}$

When latent heat: $Q_b > 0$:

1st-order phase transition.

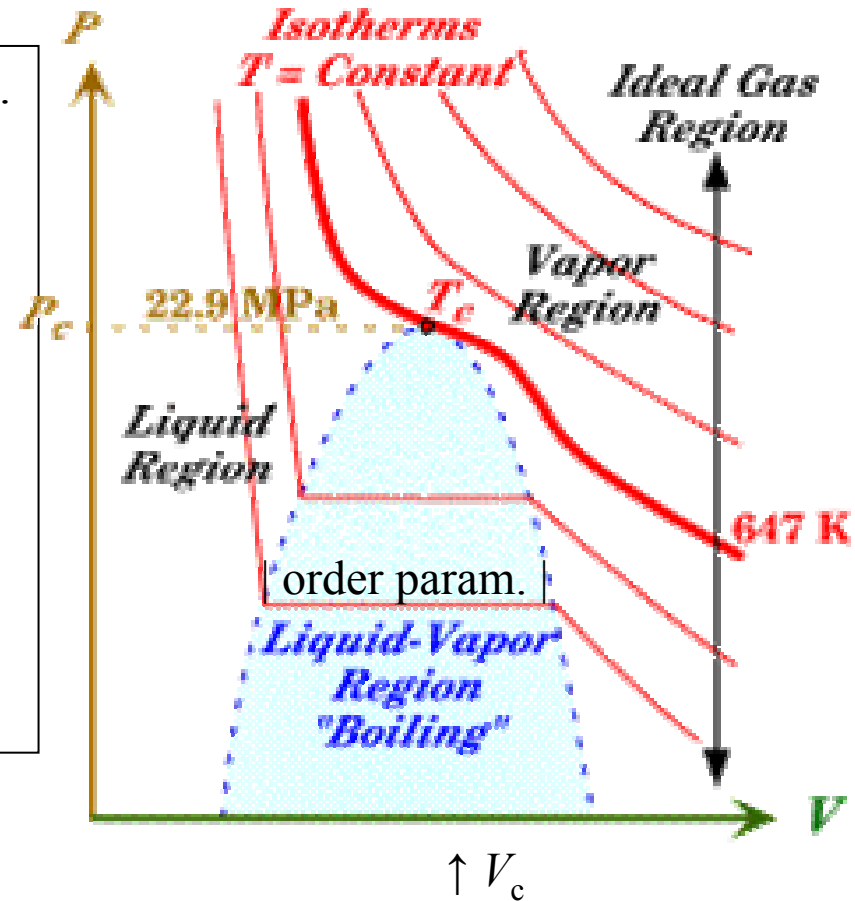
At the critical point latent heat $Q_b = 0$:

Continuous phase transition
(or 2nd order phase transition)

Boiling water:

Order parameter $= \rho_{\text{liquid}} - \rho_{\text{gas}}$

p - V phase diagram
for water (H_2O):



3. The liquid-gas transition

Equation of State:

Pressure $P = P(V, T, \dots)$

Example:

Ideal gas: $P = RT/V = \rho kT$ Gas equation

(mole volume V , density $\rho = N_A/V$, , $R = N_A k$)

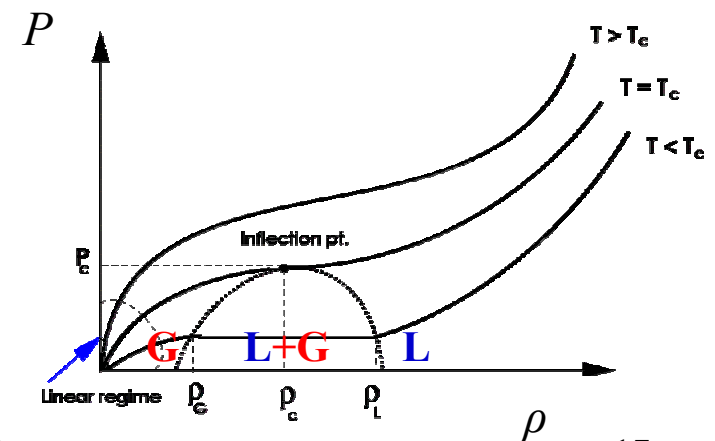
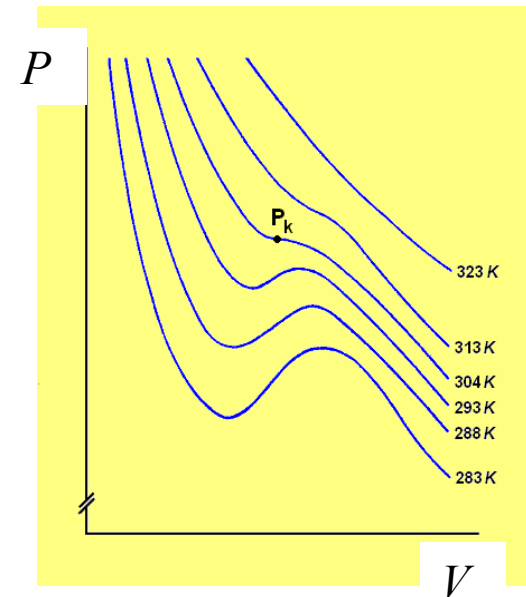
Real gas: van der Waals-equation

$$(P + a/V^2)(V - b) = RT$$

(attractive \uparrow \uparrow repulsive part
of molecular potential)

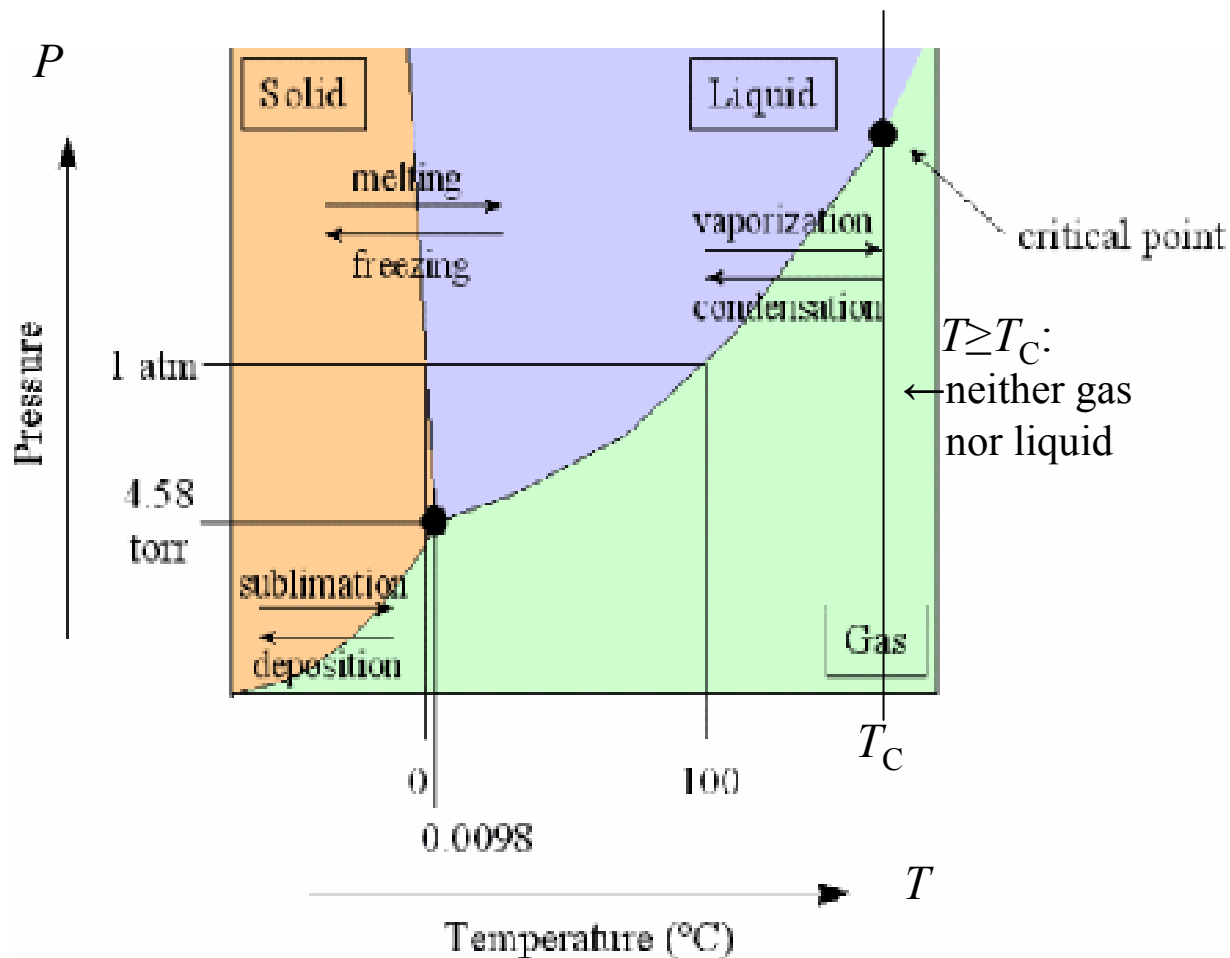
or
$$P = RT/(V - b) - a/V^2$$

same in p - ρ diagram:



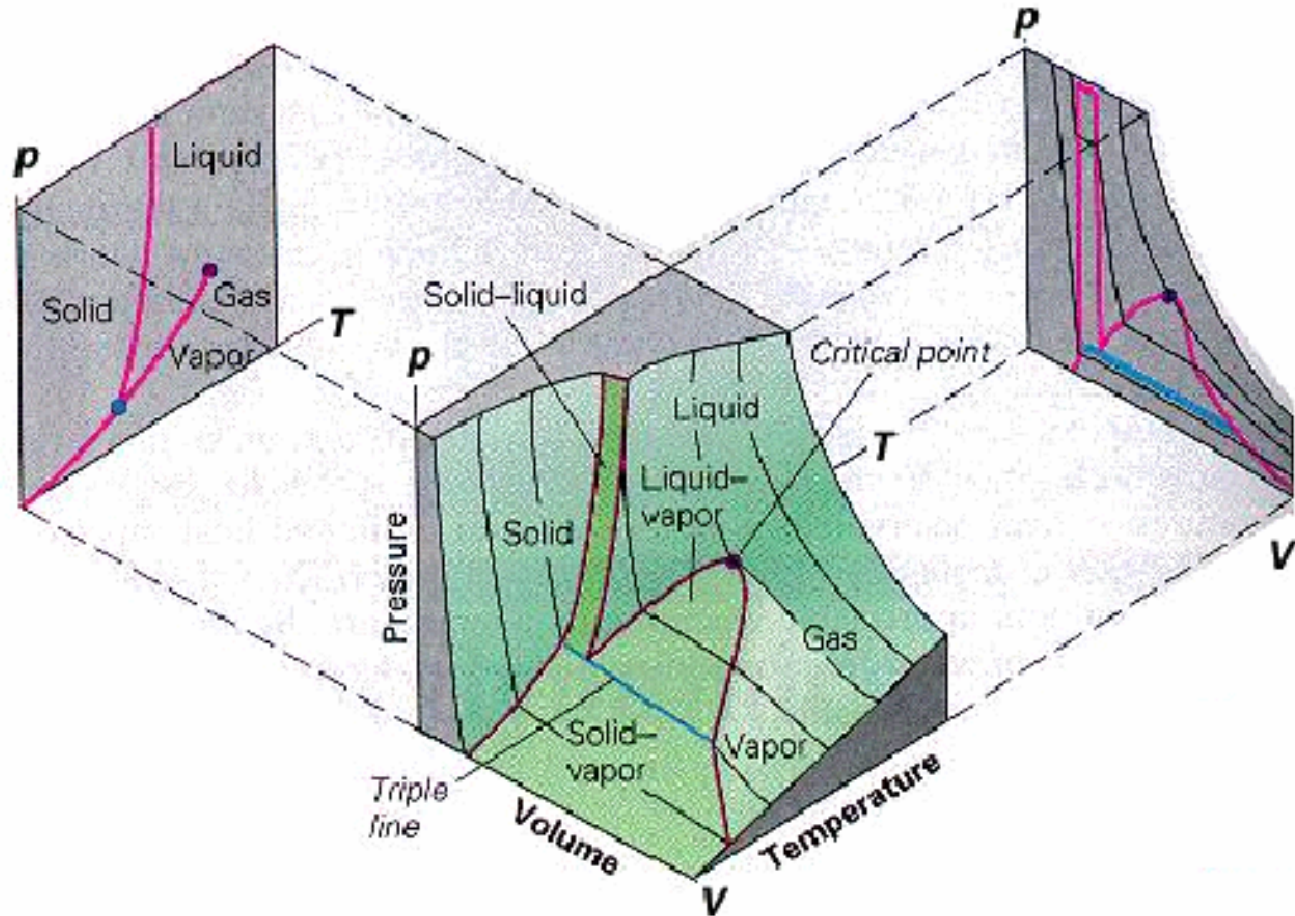
p - T phase diagram

p - T phase diagram for water (H_2O):



p - V - T phase diagram

plus various projections:
Carbon dioxide (CO_2).



Universality of the v.d.W.-equation

Bild Yeomans p. 28:

Reduced van der Waals-equation:

$$(P/P_C + 3(V_C/V)^2) (V/V_C - 1/3) = 8RT_C$$

with critical values P_C , V_C , T_C

(or $\rho_C = N_A/V_C$)

seems to be **universal**:

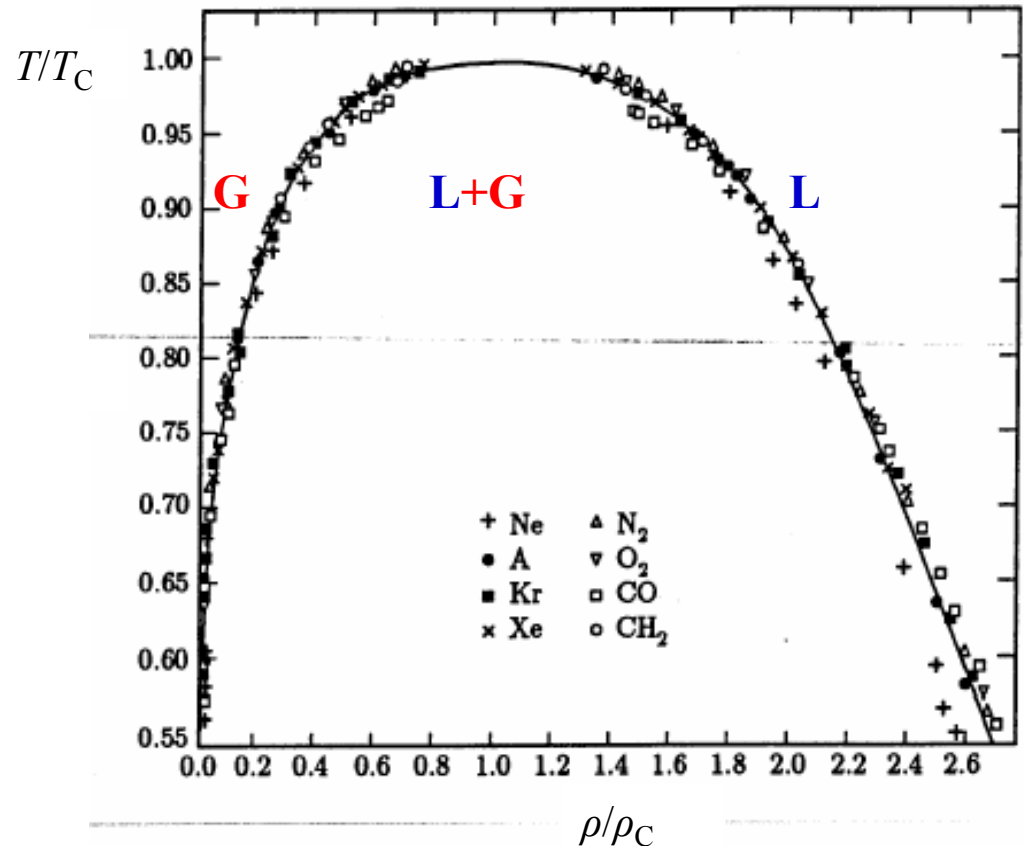


Fig. 4.4.4. Phase boundary in units of reduced temperature and density for eight different molecular fluids near their liquid-gas transitions. Note the universal behavior and the fact that the solid line is $\Delta\phi \propto (T_c - T)^\beta$ with $\beta = 1/3$ rather than the mean-field result $\beta = 1/2$. [E.A. Guggenheim, *J. Chem. Phys.* 13, 253 (1945).]

Critical exponents of v.d.Waals gas

1. Order parameter:

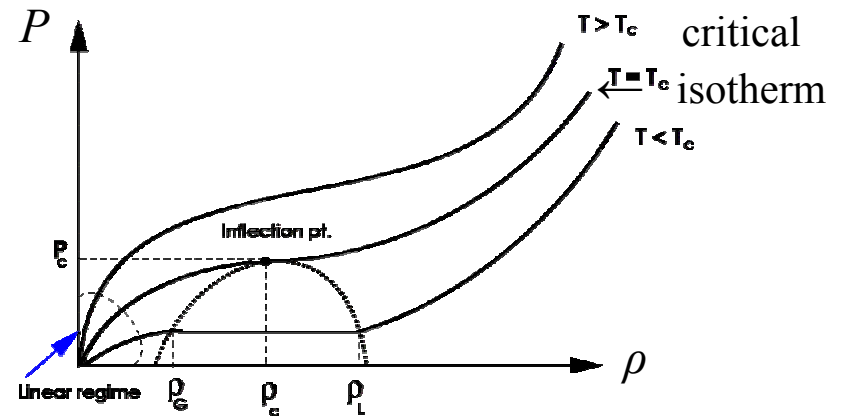
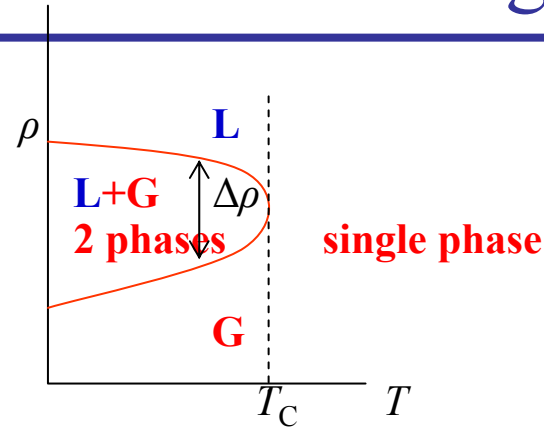
Like in the case of the ferromagnet, near $T \sim T_C$ the order parameter depends on T as: $\rho_L - \rho_G \sim (T - T_C)^\beta$ with a **critical exponent** β .

('mean field': $\beta = 1/2$)

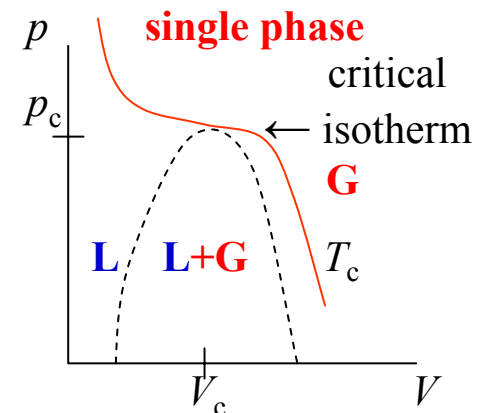
2. 'Critical isotherm':

At $T = T_C$ this isotherm is $p - p_c \sim |\rho - \rho_c|^\delta$ with a **critical exponent** δ

('mean field': $\delta = 3$)



same in p - V diagram:



More critical exponents

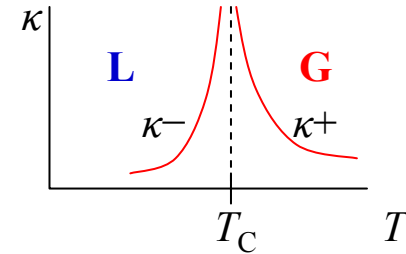
3. Compressibility $\kappa=(1/V)\partial V/\partial p$ diverges:

above T_C : $\kappa^+ \sim |T - T_C|^{-\gamma}$ **G**

below T_C : $\kappa^- = \frac{1}{2} \kappa^+$ **L**

(= 'susceptibility' against external parameter p)
with a critical exponent γ

('mean field': $\gamma = 1$)

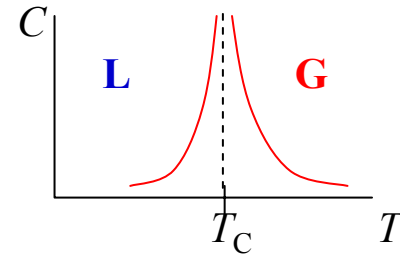


4. Specific heat diverges:

$$C \sim |T - T_C|^{-\alpha}$$

with a critical exponent α

('mean field': $\alpha = 0$)



Critical exponents from v.d.W.-equation

From a detailed inspection of the v.d.W.-equation near $T = T_C$ one finds (Domb S. 55):

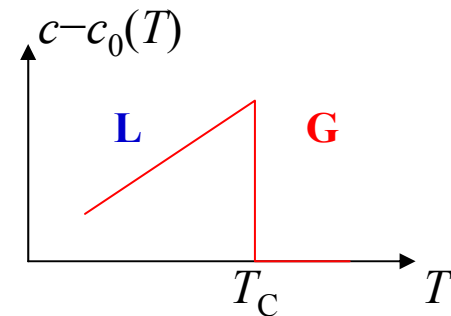
order parameter $\rho_L - \rho_G \sim (T - T_C)^{1/2}$ i.e. $\beta = 1/2$

critical isotherm $p - p_C \sim |V - V_c|^\delta$ i.e. $\delta = 3$

compressibility $\kappa \sim |T - T_C|^{-\gamma}$ i.e. $\gamma = 1$

specific heat has only discontinuity i.e. $\alpha = 0$

Lit: C. Domb, The Critical Point, Taylor and Francis 1996



Measured critical exponents

Domb p. 22:
critical isotherm has $\delta > 3$

Yeomans p. 28:
specific heat has a small $\alpha > 0$

Domb p. 206:
phase-separatrix has $\beta \approx 1/3$:

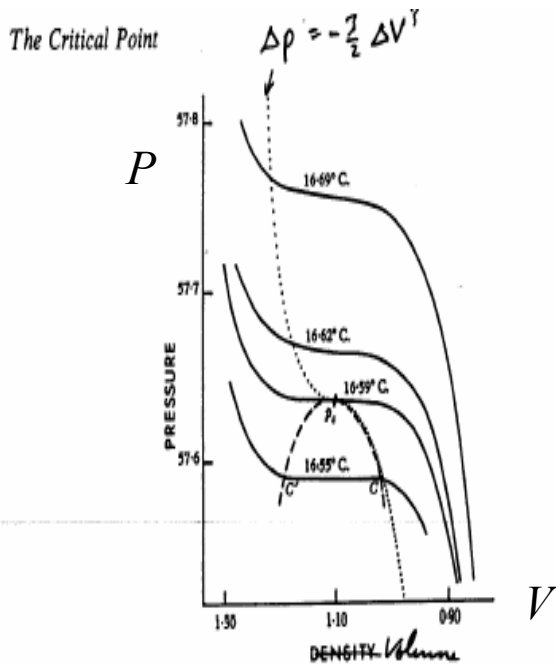


Figure 1.7 Isotherms of xenon near the critical point (Habgood and Schneider 1954). The dashed line marks the region of coexistent phases. The dotted line is the critical isotherm according to van der Waals' equation to be contrasted with the measured 16.59°C isothermal.

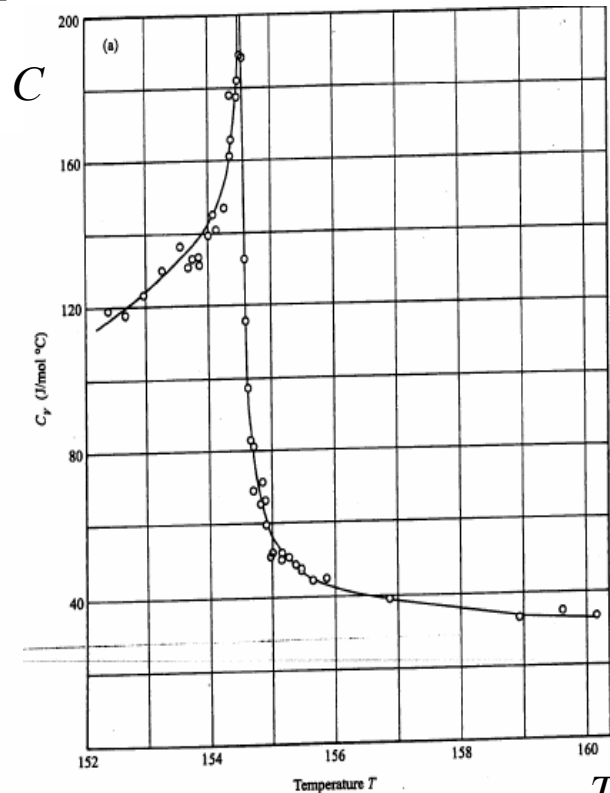


Figure 5.25 (a) Temperature dependence of C_p of oxygen at $\rho \sim \rho_c = 0.408 \text{ g/cm}^3$; (b) (opposite) dependence of C_p of oxygen on $\ln|T - T_c|$.

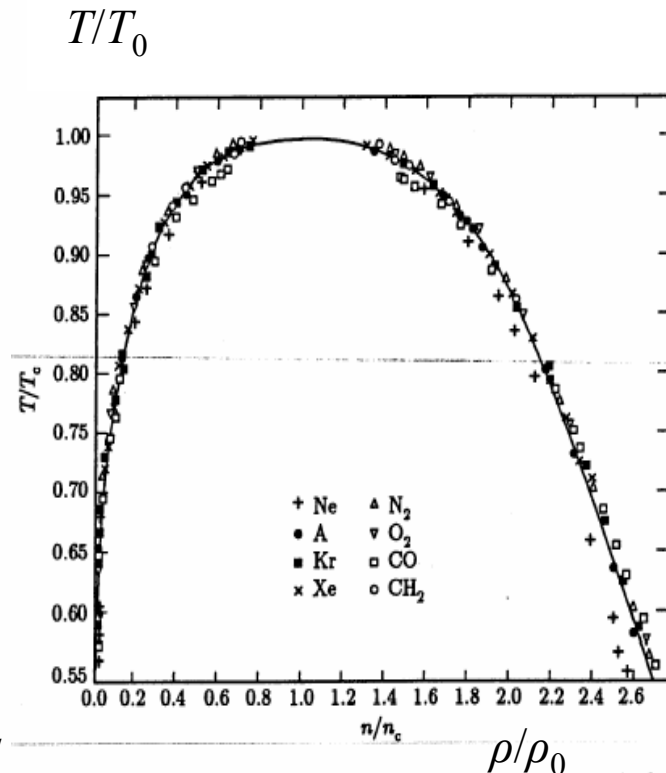


Fig. 4.4.4. Phase boundary in units of reduced temperature and density for eight different molecular fluids near their liquid-gas transitions. Note the universal behavior and the fact that the solid line is $\Delta\phi \propto (T_c - T)^\beta$ with $\beta = 1/3$ rather than the mean-field result $\beta = 1/2$. [E.A. Guggenheim, *J. Chem. Phys.* 13, 253 (1945).]

4. Thermodynamics

Internal energy: $U = \langle E \rangle = \langle E_{\text{kin}} \rangle + \langle E_{\text{pot}} \rangle,$

with temperature T defined by $kT = \langle E_{\text{kin}} \rangle$

1st law of thermodynamics: $dU = \delta Q + \delta W$

Internal energy U changes when external energy is added
either as random molecular energy, called heat Q ,
or as 'directed' macroscopic energy, called work $W = -PdV$:

$$dU = \delta Q - P dV$$

for reversible δQ : $dS = \delta Q/T$:

$$dU = T dS - P dV$$

Energy-content also changes with particle number N :

$$dU = T dS - p dV + \mu dN$$

with chemical potential $\mu = \partial U / \partial N$.

At equilibrium: $U \rightarrow \min$, i.e. $dU = 0$

only possible if $\delta Q = TdS = 0$, $dV = 0$, $dN = 0$

i.e. $Q = \text{const}$, $V = \text{const}$, $N = \text{const}$. : not very interesting

Free energy

More useful in condensed matter physics is the

Free energy: $F = U - TS \rightarrow dF = -S dT - P dV + \mu dN$ (physics)

At equilibrium: $F \rightarrow \min$, i.e. $dF = 0$:

$T = \text{const}$, $V = \text{const}$, $N = \text{const}$, but heat exchange $\delta Q \neq 0$ is permitted.

Taylor:
$$dF = \frac{\partial F}{\partial T} dT + \frac{\partial F}{\partial V} dV + \frac{\partial F}{\partial N} dN$$
 (mathematics)

From comparison of both one finds:

From a given free energy $F = F(T, V, N)$ all state variables can be obtained:

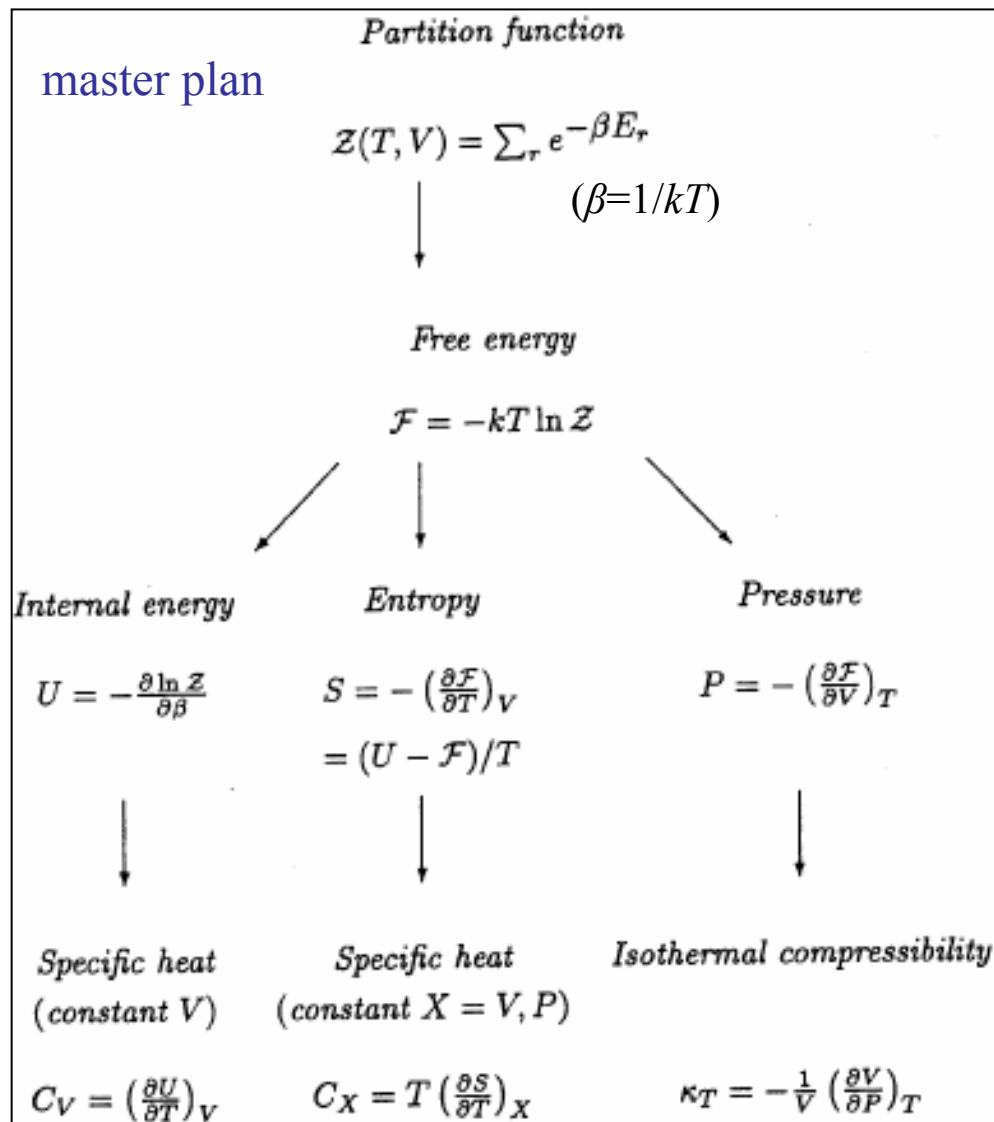
Entropy $S = -\partial F / \partial T$

Pressure $P = -\partial F / \partial V = P(T, V, N) = \text{equation of state}$

Chemical potential $\mu = \partial F / \partial N, \dots$

From free energy → everything else

master plan



More precisely:

From

Partition function (more later)

$$Z = \sum_r \exp(-E_r/kT)$$

or

$$Z = \iint_{\text{phase space}} " "$$

summed over all possible states with energies E_r .

Same 'master plan' for magnetism

In solid: $dV \approx 0$.

With magnetic field B (or H):

Free energy

$$dF = -SdT - MdB$$

i.e. $F = F(T, B)$

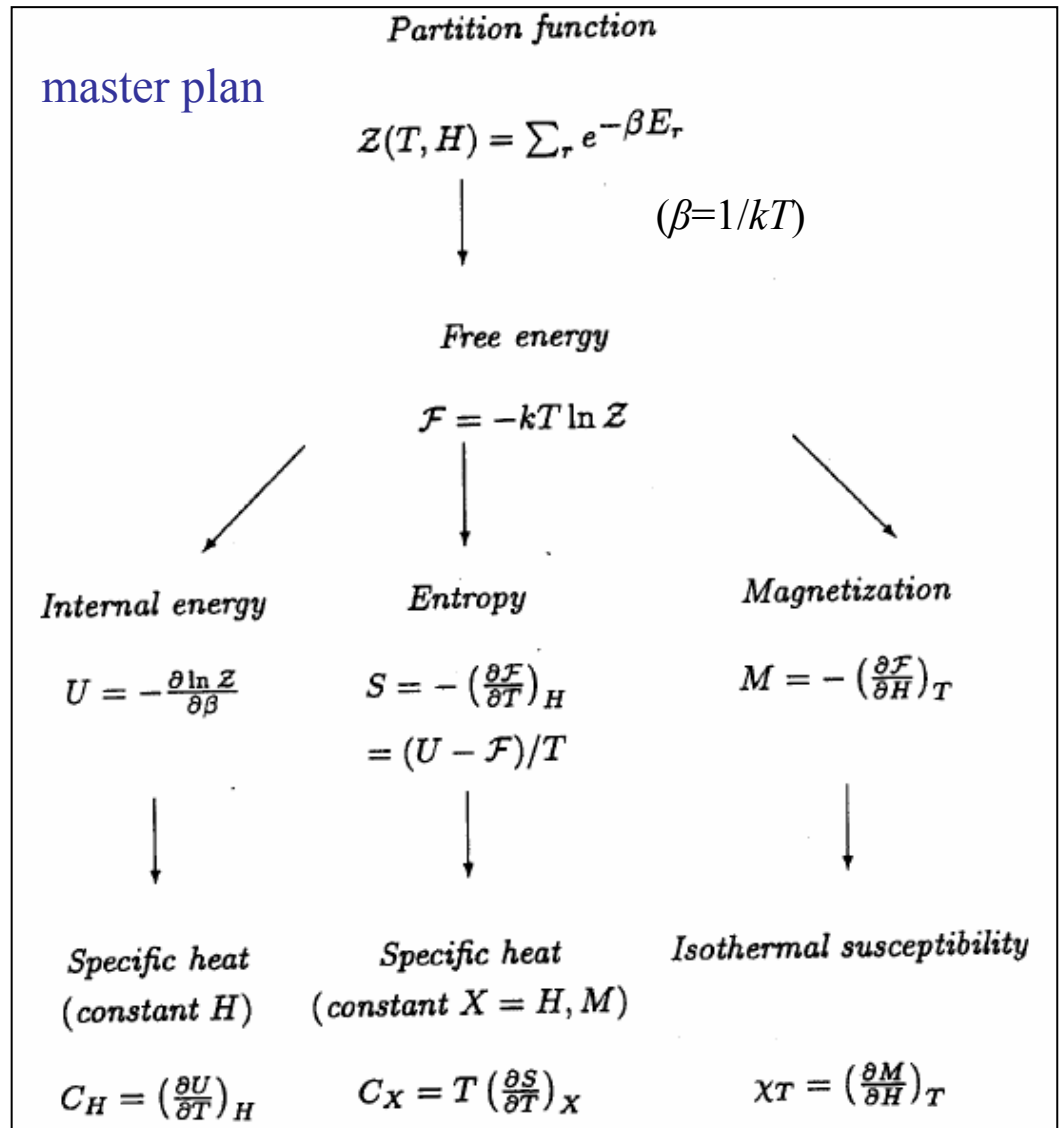
with magnetization

$$M = -\partial F / \partial B,$$

and magn. susceptibility

$$\chi = \partial M / \partial B$$

Yeomans p.17:



Example paramagnetism

Hamiltonian $\hat{H} = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu B$ for $B=B_z$ and magnetic moment μ
 spin $1/2$ -system with two states for each molecule:

energy/molecule $E_{\pm} = \pm\mu B$

partition function for N molecules:

$$Z = \left(\sum_r e^{-\beta E_r} \right)^N = (e^{-\beta E_+} + e^{-\beta E_-})^N \quad \beta = 1/kT$$

magnetisation

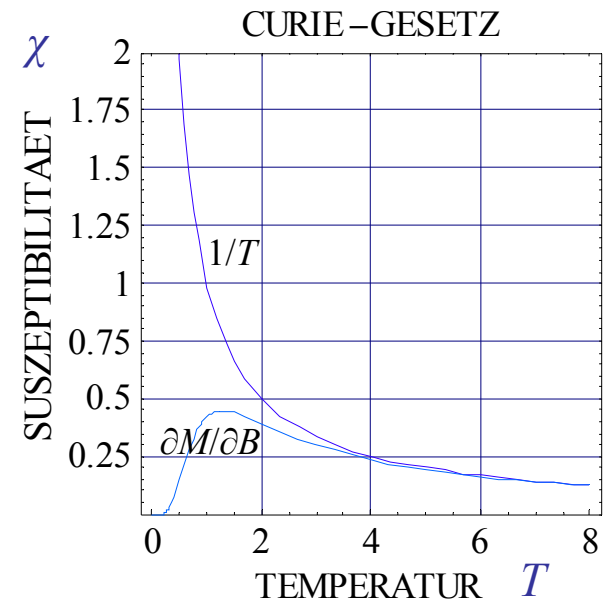
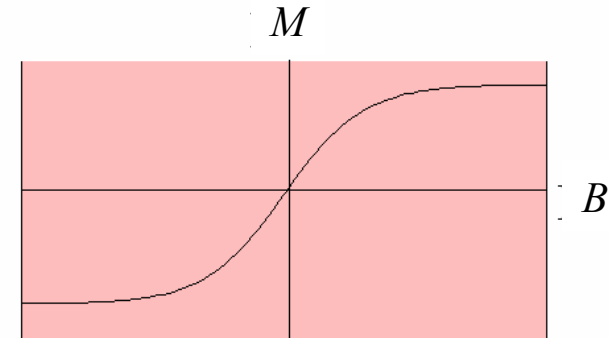
$$\langle M \rangle = NkT \frac{1}{Z} \frac{\partial Z}{\partial B} = M_0 \frac{e^{-\beta E_+} - e^{-\beta E_-}}{e^{-\beta E_+} + e^{-\beta E_-}}$$

$$\langle M \rangle = N\mu \tanh\left(\frac{\mu B}{kT}\right) \approx \frac{\mu B}{kT}$$

Saturation magnetis. $M_0 = N\mu$

Susceptibility $\chi = \partial M / \partial B \approx N\mu^2 / kT$: $\chi \sim 1/T$
 = Curie Law, for $kT \gg \mu B$

PM:



5. Landau model of magnetism

Landau 1930

Lit: Landau Lifschitz 5: Statistical Physics ch. XIV

'Landau' free energy of ferromagnet $F = F(m)$

with magnetization $m = \langle M \rangle / M_0$ (mean field approx.)

(or any other continuous phase transition)

Order parameter m Taylor-expanded about $m=0$:

$$F = F_0(T) + (\frac{1}{2}a' m^2 + \frac{1}{4}\lambda m^4)V$$

has only even powers of m , as F does not depend on sign of m ,
 $\lambda > 0$ to contain system.

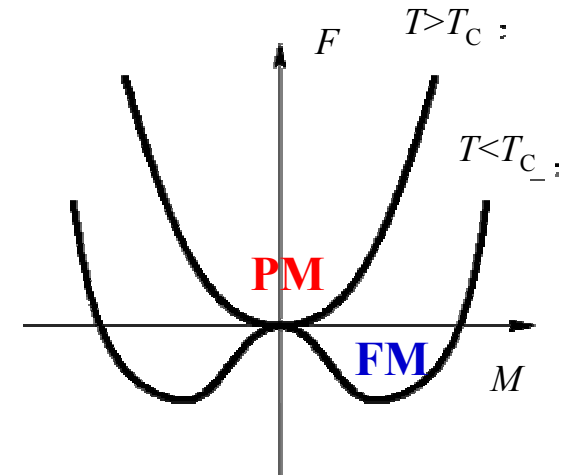
Assume a' changes sign at $T=T_C$ (linear approx.)

$$a' = a \cdot (T - T_C)$$

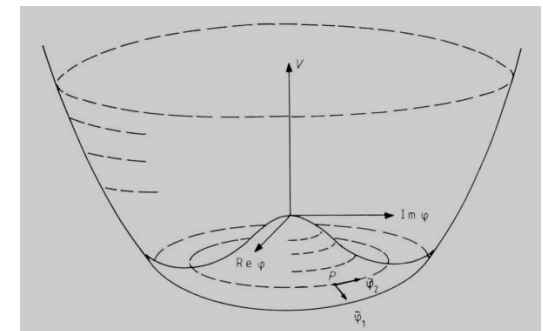
Free energy density $f = (F - F_0)/V$ then is:

$$f = \frac{1}{2}a(T - T_C) m^2 + \frac{1}{4}\lambda m^4$$

1-dim magnet:



2-dim magnet:



Spontaneous magnetization in zero external field

Landau: $f = \frac{1}{2}a(T - T_C) m^2 + \frac{1}{4}\lambda m^4$ phase diagram $h-T$:

At equilibrium \rightarrow minimum of free energy:

$$\partial f / \partial m = a(T - T_C) m + \lambda m^3 = 0$$

1st solution order param. $m = 0$:

extremum of f is a minimum only for $T \geq T_C$: **PM**

2nd solution: $m = \pm(a/\lambda)^{1/2}(T_C - T)^{1/2}$ (1)

m is real only for $T < T_C$: **FM**

has critical exponent $\beta = 1/2$.

Same result as for order parameter of v.d.W. gas:

$$\rho_L - \rho_G \sim (T_C - T)^{1/2}.$$

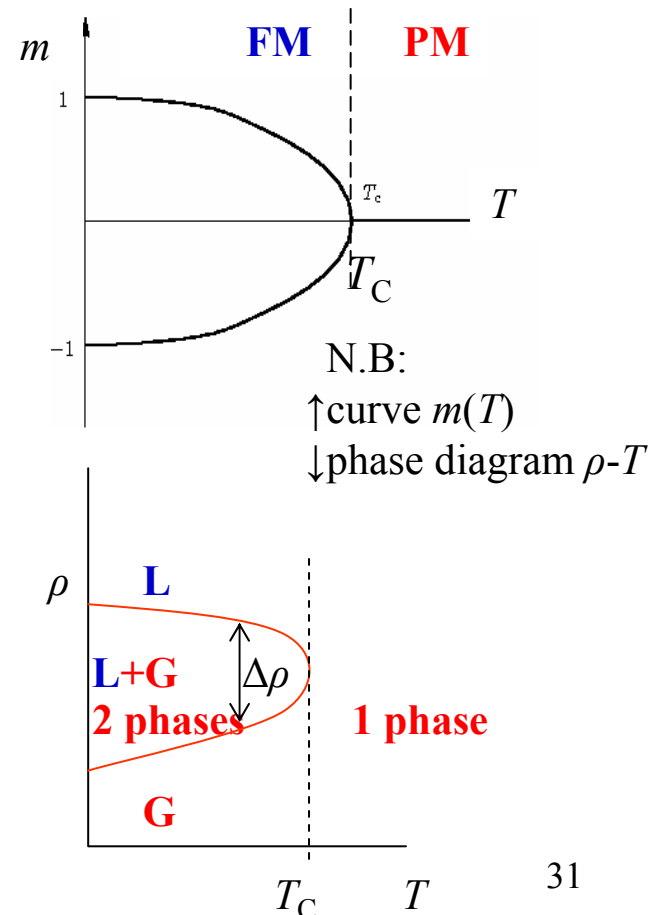
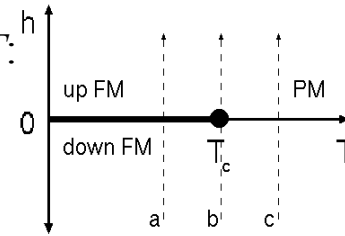
N.B.: above T_C : high symmetry, group S

below T_C : lower symmetry, group S'.

necessarily: S' = subgroup of S

(see Landau Lifschitz 5 §145)

"spontaneous breaking of symmetry"



Magnetization in external field

Magnetic energy in external magnetic field B :

$$f_M = -BM = -hm \text{ with field parameter } h = BM_0$$

i.e.: $f = \frac{1}{2}a(T-T_C) m^2 + \frac{1}{4}\lambda m^4 - hm$

At equilibrium: from

$$\partial f / \partial m = a(T-T_C) m + \lambda m^3 - h = 0 \quad (2)$$

follows magnetization $\pm m(T)$, see Fig., in particular:

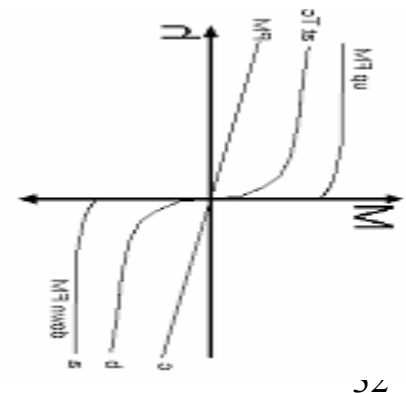
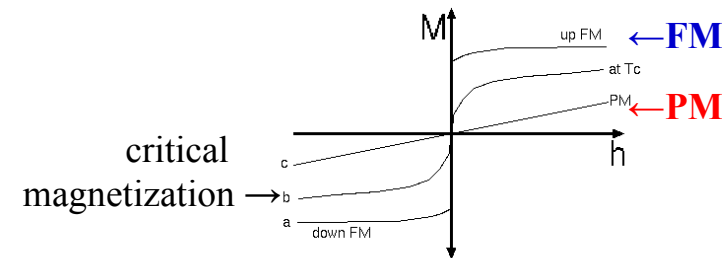
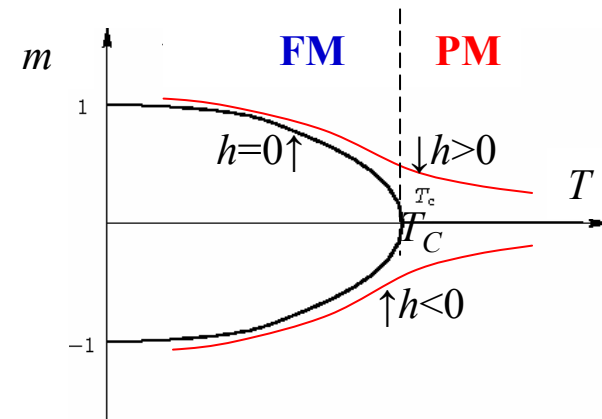
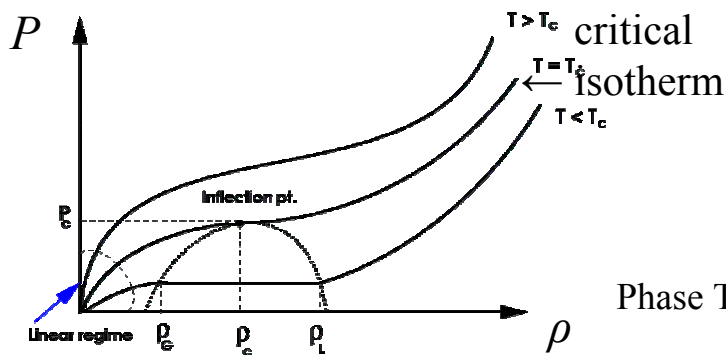
critical magnetization at $T = T_C$:

$$h = \lambda m^3$$

has critical exponent $\delta = 3$.

Similar result as for critical isotherm of v.d.W. gas:

$$p - p_C \sim |\rho - \rho_C|^3, \text{ see below:}$$



Magnetic susceptibility

Susceptibility $\chi = \partial m / \partial h$ diverges at $T = T_C$.

Proof: At equilibrium, from (2):

$$\phi(m) \equiv a(T - T_C) m + \lambda m^3 = h$$

$$\partial \phi / \partial h = (\partial \phi / \partial m) \cdot (\partial m / \partial h) =$$

$$(a(T - T_C) + 3\lambda m^2) \chi^+ = 1 \quad (3)$$

above T_C : $m = 0$ in (3): $a(T - T_C) \chi^+ = 1$

$\chi^+ = [a(T - T_C)]^{-1}$ Curie-Weiss law **PM**

has critical exponent $\gamma = 1$

below T_C : $m^2 = (a/\lambda)(T_C - T)$ from (1), in (3):

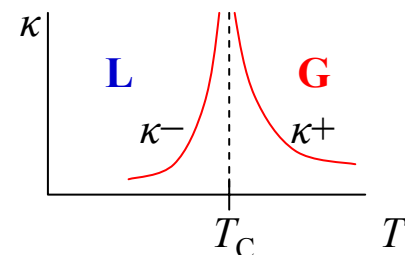
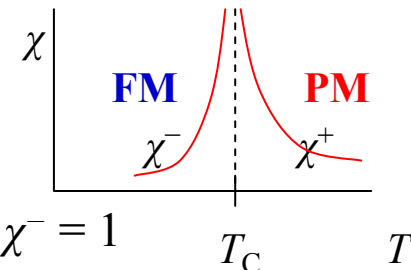
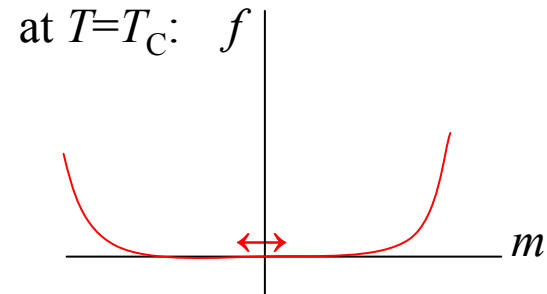
$$[-a(T_C - T) + 3\lambda (a/\lambda)(T_C - T)] \chi^- = [2a(T_C - T)] \chi^- = 1$$

$$\chi^- = [2a(T_C - T)]^{-1} = \frac{1}{2} \chi^+.$$

Curie-Weiss law **FM**

Same result as for v.d.W.-compressibility κ^- and κ^+ :

Reason: Free energy has flat bottom



Specific heat in zero field

Value of energy density $f = \frac{1}{2}a(T - T_C) m^2 + \frac{1}{4}\lambda m^4$
at its minimum (i.e. in equilibrium):

above T_C : $m = 0 \rightarrow f = 0$

below T_C : $m^2 = (a/\lambda)(T_C - T)$ from (1) \rightarrow
 $f = -\frac{1}{2}(a^2/\lambda)(T_C - T)^2$

Entropy is lowered linearly below T_C :

above T_C : $s - s_0(T) = -\partial f/\partial T = 0$ **PM**

below T_C : $s - s_0(T) = -(a^2/\lambda)(T_C - T)$ **FM**

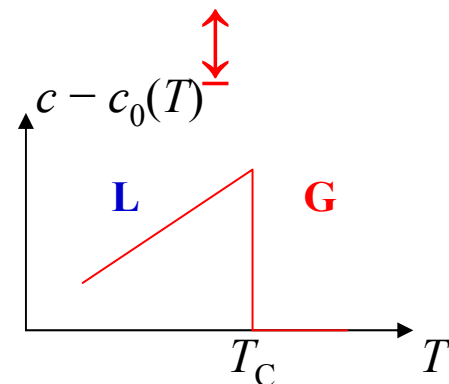
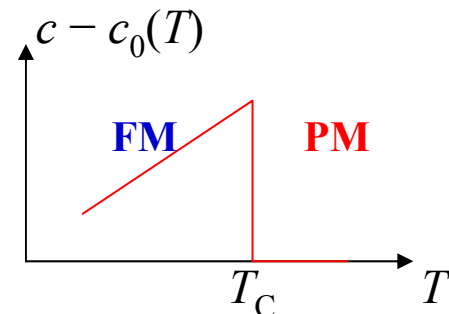
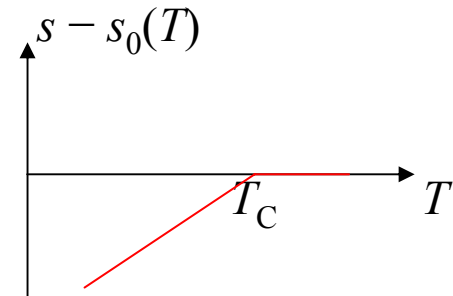
Specific heat makes a jump at T_C :

above T_C : $c - c_0(T) = -\partial s/\partial T = 0$ **PM**

below T_C : $c - c_0(T) = -T \partial s/\partial T = (a^2/\lambda)T$ **FM**

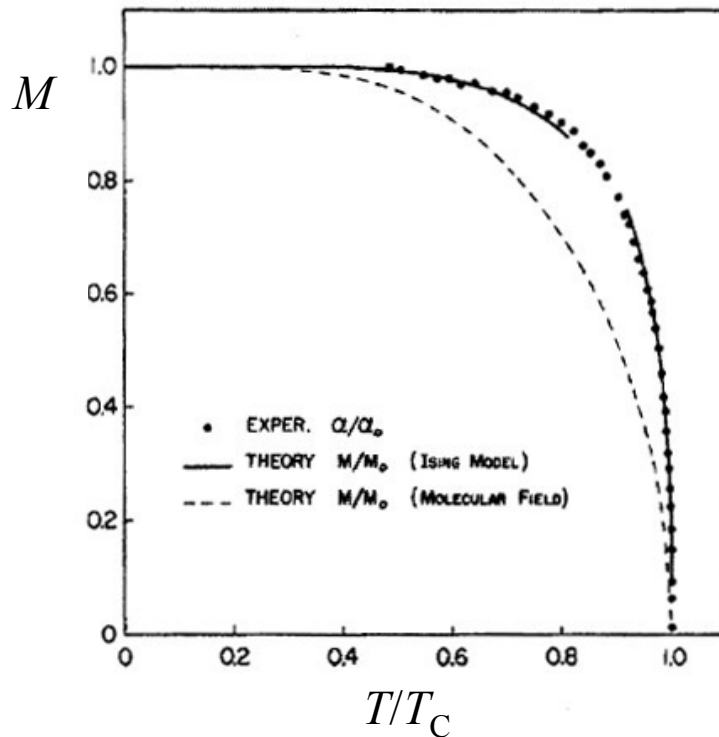
i.e. has critical exponent $\alpha = 0$.

Same result as for specific heat of v.d.W. gas:

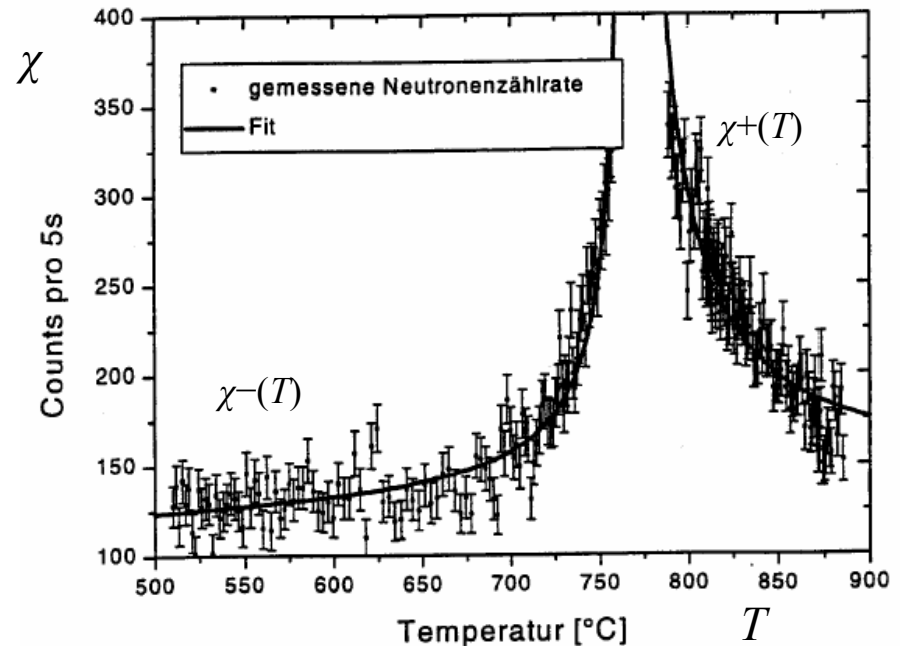


Compare with experiment

Magnetization: $M \sim (T_C - T)^\beta$



Susceptibility: $\chi^+(T) \sim (T - T_C)^{-\gamma}$
 $\chi^-(T) = \frac{1}{2} \chi^+(T)$



Landau or

	α	β	γ	δ
VdW	0	1/2	1	3
Exp.	0.1	0.34	1.35	4.2

Example: magnetic phases

Yeomans S. 6

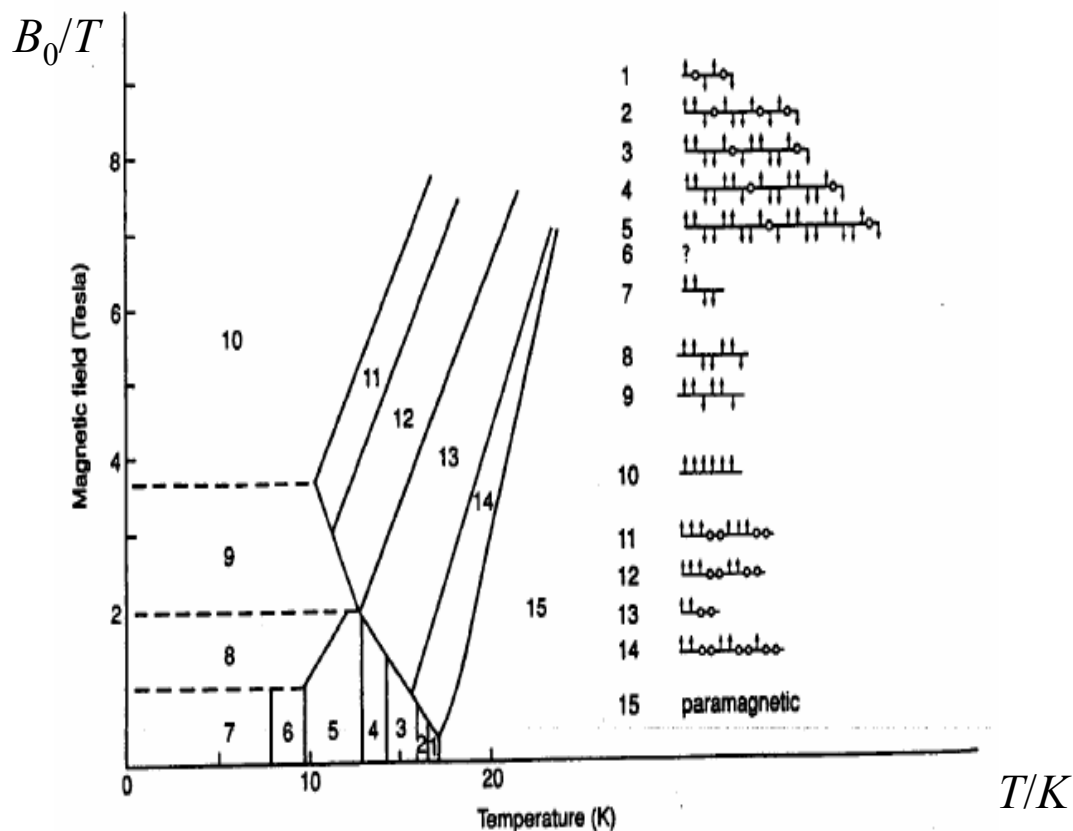


Fig. 1.6. The ferrimagnetic phases of cerium antimonide. The relative ordering of successive ferromagnetic planes in each phase is indicated in the Figure. o denotes a plane with a net magnetization of zero

Related: catastrophe theory

Arnol'd-classification of different types of catastrophes is due to a deep connection with simple Lie groups:

A_0 - a non singular point

A_1 - a local extrema, either a stable minimum or unstable maximum

A_2 - the fold \leftrightarrow van der Waals:

A_3 - the cusp

A_4 - the swallowtail

A_5 - the butterfly

A_k - an infinite sequence of one variable forms

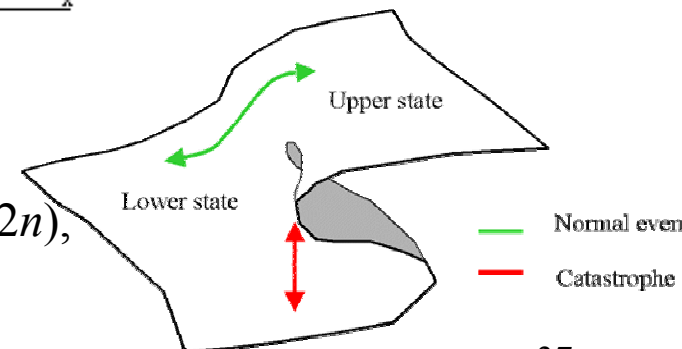
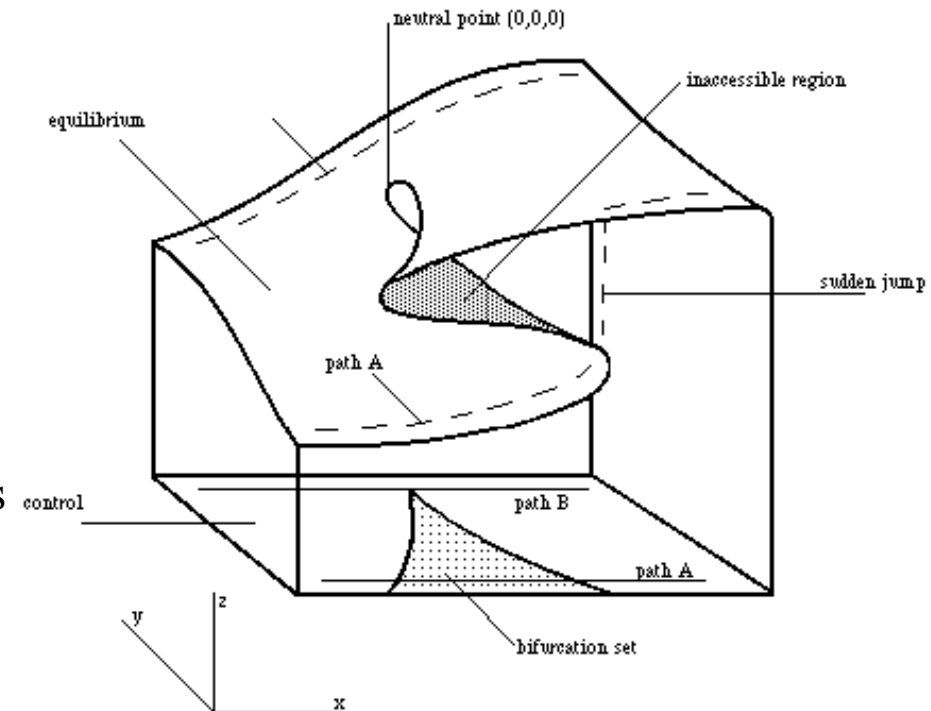
D_4 - - the elliptical umbilic

D_4^+ - the hyperbolic umbilic

D_5 - the parabolic umbilic

D_k - an infinite sequence of further umbilic for...

E_6 - the symbolic umbilic

 E_7, E_8 

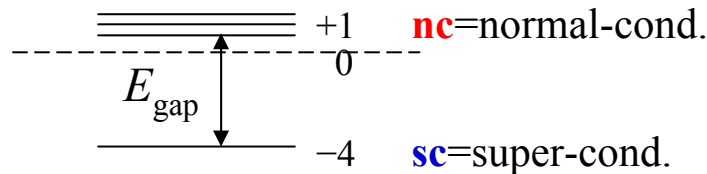
Here A_n is the algebra of $SU(n+1)$; D_n is the algebra of $SO(2n)$, while E_k are three of five exceptional compact Lie algebras.

6. Ginzburg-Landau theory of superconductivity

'Microscopic' BCS theory: Energy gap induced by attractive electron-electron interaction

(mock-BCS, from Kittel: Solid State Physic, Appendix E): $\hat{H}V = EV$, i.e.

$V^\dagger \hat{H} V = E$, with:

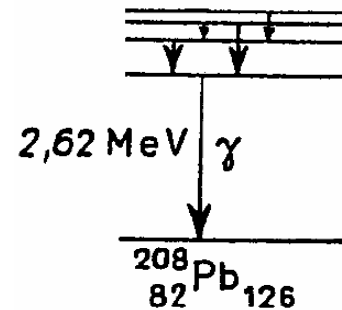


$$\hat{H} = - \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

5 electrons →
e
l
e
c
t
r
o
n
s
↓

Energy gap induced by attractive nucleon-nucleon interaction

(from Maier-Kuckuck: Kernphysik p. 68):



$E =$ Energy-
Eigenvalues |
sc ↓ **nc**
 $\{-4, 1, 1, 1, 1\}$
= diagonal matrix

Electron-
Eigenvectors
 $\{1, 1, 1, 1, 1\} \leftarrow \text{sc}$

$V =$

$\{-1, 0, 0, 0, 1\}$	} nc
$\{-1, 0, 0, 1, 0\}$	
$\{-1, 0, 1, 0, 0\}$	
$\{-1, 1, 0, 0, 0\}$	

Cooper pairs:

charge $e^* = 2e$

mass $m^* = 2m_e$

density $|\psi|^2 = n_s/2$,

with **complex** $\psi(\mathbf{r}) = (n_s/2)^{1/2} e^{i\theta(\mathbf{r})}$

(n_s = density of superconducting electrons = 2×density of Cooper pairs)

Homogeneous superconductor in zero field

In superconductivity, the 'macroscopic' mean field approximation is valid to temperatures very close to T_c , as $\psi(\mathbf{r})$ of a Bose condensate cannot fluctuate strongly.

a) without magnetic field $B = 0$,

density of s.c. electrons $n_s = \text{const.}$ in volume V

Landau free energy near T_c (with F_n for normal conduction):

$$F_s = F_n + (\frac{1}{2}a \cdot (T - T_c) |\psi_s|^2 + \frac{1}{4}\lambda |\psi_s|^4) V$$

with order parameter $\psi_s \sim n_s^{1/2}$, transition temperature T_c .

From $\partial F_s / \partial \psi_s = 0$, the density of s-c electrons in the minimum is:

above T_c : $n_s = |\psi_s|^2 = 0$ **nc**

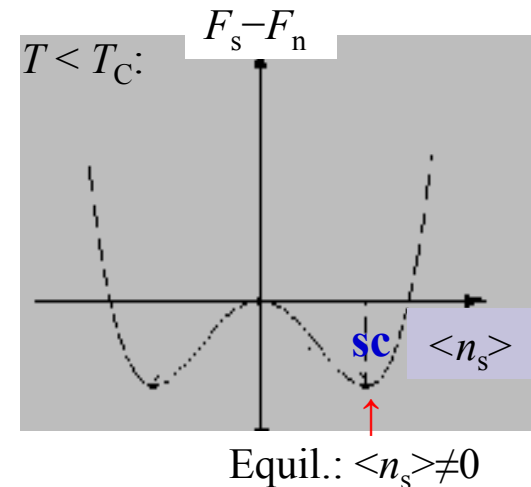
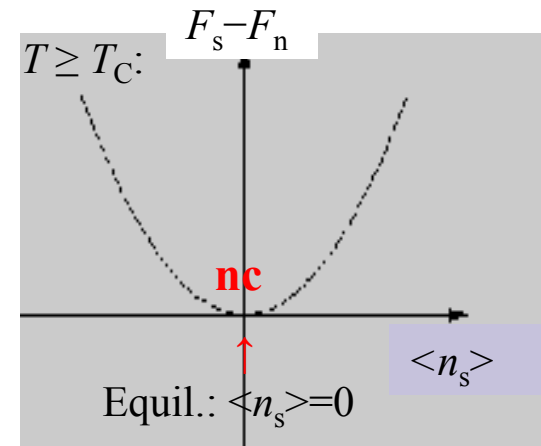
below T_c : $n_s = |\psi_s|^2 = (a/\lambda)(T_c - T)$ **sc**

At minimum, the value of F is:

above T_c : $F_s = F_n$ **nc**

below T_c : $F_s = F_n - \frac{1}{4}(a^2/\lambda)(T_c - T)^2 V$ **sc**

In the **sc**-state the free energy is lowered (s-cond. energy gap)



Critical magnetic field B_c

b) with magnetic field $B \neq 0$:

Energy density of the field is $B^2/2\mu_0$.

If magnetic field energy is so large that $F_s > F_n$,
then superconductivity disappears:

$$F_s = F_n - (a^2/4\lambda)(T_C - T)^2 V + (B^2/2\mu_0)V > F_n$$

This the case when B surpasses the critical field

$$B_C = a(\mu_0/2\lambda)^{1/2}(T_C - T) \quad (\text{near } T_C). \quad (4)$$

Experiment: down to $T=0$, B_C can be approximated by

$$B_C \approx B_{C0}(1 - T^2/T_C^2) = B_{C0}(1 - T/T_C)(1 + T/T_C)$$

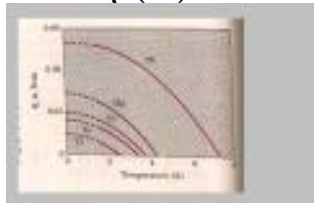
which is $\approx 2B_{C0}(T_C - T)/T_C$ near T_C .

Comparison with (4) gives the pre-factor,
the zero-temperature critical field

$$B_{C0} = \frac{1}{2}(\mu_0/2\lambda)^{1/2} a T_C,$$

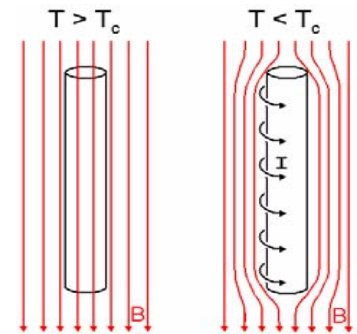
that is the whole $B_C(T)$ curve grows linearly with T_C .

Experiment:

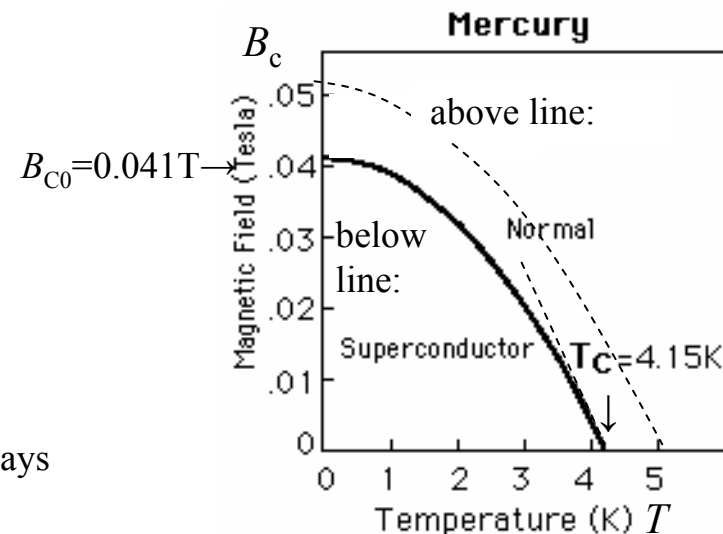


Phase Transitions Graduate Days
Oct. 2006

Meissner Effect:



Phase diagram:



Non-uniform superconductor in zero field

In general a superconductor is not uniform (mixed phases, Meissner effect, etc.):
order parameter is position dependent: $\psi = \psi(\mathbf{r})$. (short: ψ for ψ_s).

If free-energy F is at its minimum for a constant ψ_0 ,
i.e. F is minimum with respect to all possible variations $\nabla\psi$,
then deviations from ψ_0 must be quadratic in $\nabla\psi$ (like in elasticity theory),
i.e. the energy penalty for deviations from homogeneity is $\sim |\nabla\psi|^2$.

a) without magnetic field $B = 0$:

$$F_s = F_n + \int_V \left(+(\hbar^2/2m^*) |\nabla\psi|^2 + \frac{1}{2}a \cdot (T - T_c) |\psi|^2 + \frac{1}{4}\lambda |\psi|^4 \right) dV$$
$$F_{\text{sc}} = F_{\text{nc}} + \quad T_{\text{sc}} = E_{\text{sc kin}} \quad + \quad V_{\text{sc}} = E_{\text{sc pot}}$$

where the constants have been adjusted so
the transition to quantum mechanics becomes evident.

Non-uniform superconductor in magnetic field

b) with magnetic field:

$\mathbf{B} = \mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, with vector potential \mathbf{A} ,

\mathbf{A} changes momentum $m\mathbf{v}$ of a particle to

$$\mathbf{p} = m\mathbf{v} + e\mathbf{A}$$

but does not change its energy

$$E = (m\mathbf{v}^2)/2m = (\mathbf{p} - e\mathbf{A})^2/2m$$

therefore for $\mathbf{B} \neq 0$ (Ginzburg-Landau, 1950):

$$F_s = F_n + \int_V (| -i\hbar \nabla \psi_s - e^* \mathbf{A} \psi_s |^2 / 2m^* + \frac{1}{2} a \cdot (T - T_c) |\psi_s|^2 + \frac{1}{4} \lambda |\psi_s|^4 + \mathbf{B}^2 / 2\mu_0 - \mathbf{B} \cdot \mathbf{M}) dV$$

$$F_{\text{sc}} = F_{\text{nc}} + T_{\text{sc}} + V_{\text{sc}} + E_{\text{field}} + E_{\text{magn}}$$

$$m^* = 2m_e, e^* = 2e$$

Lit.: C.P. Poole et al.: Superconductivity, ch.5, Academic Press 1995

Two Ginzburg equations

Minimum of F_s by variational calculation: functional derivatives give

1st Ginzburg equation $\partial F_s / \partial \psi = 0$

2nd Ginzburg equation $\partial F_s / \partial A = 0$

= two coupled differential equations (see 'small print' next page)

Here we treat only a few special cases:

plane superconductor with surface in y - z plane:

a) without magnetic field $B = 0$:

1st Ginzburg-equation gives the spatial dependence of s.c. amplitude $\psi(x)$:

$$\partial F_s / \partial \psi = (\hbar^2 / 2m^*) d^2 \psi / dx^2 + a(T - T_C) \psi + \lambda \psi^3 = 0$$

= differential eq. of the type $y'' + y(1 - y^2) = 0$,

with solution: $y = \tanh x$,

from: B. Schmidt, Physics of Supercond., p. 48ff:

operator $-i\hbar\nabla$ in the expression for the kinetic energy density has to be modified:

$$-i\hbar\nabla \rightarrow -i\hbar\nabla - \frac{e}{c} \mathbf{A} = m\mathbf{v}.$$

Therefore, the velocity operator is

$$\mathbf{v} = -(i\hbar/m)\nabla - (e/cm)\mathbf{A}.$$

Since it is the velocity \mathbf{v} that enters the expression for the kinetic energy density, we can now understand why the corresponding term in (3.7) looks as it does. It should only be added that a substitution $e \rightarrow 2e$ has been made in (3.7) which takes into account that the elementary charge carrier of the supercurrent is $2e$. Accordingly, m^* in (3.7) is twice the electron mass.

3.2.2 Ginzburg-Landau (GL) Equations

By (3.7), the Gibbs free energy of a superconductor as a whole is

$$\mathcal{G}_H = \mathcal{G}_n + \int \left[\alpha |\Psi|^2 + \frac{\beta}{2} |\Psi|^4 + \frac{1}{4m} \left| -i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right|^2 + \frac{(\text{curl } \mathbf{A})^2}{8\pi} - \frac{(\text{curl } \mathbf{A}) \cdot \mathbf{H}_0}{4\pi} \right] dV, \quad (3.8)$$

where the integration is carried out over the entire volume of the superconductor. Our task now is to find equations for the functions $\Psi(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ such that their solutions, when substituted in (3.8), give the minimum value of \mathcal{G}_H .

In order to do that we shall first assume that $\Psi(\mathbf{r})$ and $\mathbf{A}(\mathbf{r})$ are invariant and then solve the variational problem with respect to $\Psi^*(\mathbf{r})$:

$$\delta_{\Psi^*} \mathcal{G}_H = 0, \quad (3.9)$$

$$\delta_{\Psi^*} \mathcal{G}_H = \int dV \left[\alpha \Psi \delta\Psi^* + \beta \Psi |\Psi|^2 \delta\Psi^* + \frac{1}{4m} \left(i\hbar\nabla \delta\Psi^* - \frac{2e}{c} \mathbf{A} \delta\Psi^* \right) \cdot \left(-i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right) \right]. \quad (3.10)$$

The term $\delta\Psi^*$ could be taken out of the square brackets but for the term $i\hbar\nabla \delta\Psi^*$. Let us make some modifications. We write

$$\varphi = \left(-i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right).$$

Using the identity

$$\nabla(\delta\Psi^* \varphi) = \varphi \nabla \delta\Psi^* + \delta\Psi^* \nabla \varphi,$$

we then have

$$\int dV \nabla \delta\Psi^* \varphi = - \int \delta\Psi^* \nabla \varphi dV + \int \nabla(\delta\Psi^* \varphi) dV. \quad (3.11)$$

By Gauss's theorem, the last integral in (3.11) can be converted into a surface integral:

$$\int \nabla(\delta\Psi^* \varphi) dV = \oint_S \delta\Psi^* \varphi dS.$$

Substituting (3.11) into (3.10) and (3.10) into (3.9), we obtain

$$\begin{aligned} \delta_{\Psi^*} \mathcal{G}_H &= \int dV \left[\alpha \Psi + \beta \Psi |\Psi|^2 + \frac{1}{4m} \left(-i\hbar\nabla - \frac{2e}{c} \mathbf{A} \right)^2 \Psi \right] \delta\Psi^* \\ &\quad + \oint_S \left[-i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right] \delta\Psi^* dS = 0. \end{aligned}$$

For an arbitrary function $\delta\Psi^*$, this expression can be zero only if both expressions in square brackets are zero. From this requirement we obtain the first equation of the GL theory and its boundary condition:

$$\begin{aligned} \alpha \Psi + \beta \Psi |\Psi|^2 + \frac{1}{4m} \left(i\hbar\nabla + \frac{2e}{c} \mathbf{A} \right)^2 \Psi &= 0, \\ \left(i\hbar\nabla\Psi + \frac{2e}{c} \mathbf{A}\Psi \right) \cdot \mathbf{n} &= 0, \end{aligned} \quad (3.12)$$

where \mathbf{n} is the unit vector normal to the surface of the superconductor. One can easily verify that minimization of \mathcal{G}_H with respect to Ψ leads to the complex-conjugate of (3.12). Thus, we have obtained the equation for the order parameter Ψ . One variable still remains: \mathbf{A} . In order to obtain the equation for \mathbf{A} , we shall minimize the expression for \mathcal{G}_H (3.8) with respect to \mathbf{A} :

$$\begin{aligned} \delta_{\mathbf{A}} \mathcal{G}_H &= \int dV \left\{ \frac{1}{4m} \delta_{\mathbf{A}} \left[\left(i\hbar\nabla\Psi^* - \frac{2e}{c} \mathbf{A}\Psi^* \right) \cdot \left(-i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right) \right] \right. \\ &\quad \left. + \frac{1}{4\pi} \text{curl } \mathbf{A} \cdot \text{curl } \delta\mathbf{A} - \frac{\mathbf{H}_0}{4\pi} \cdot \text{curl } \delta\mathbf{A} \right\} \\ &= \int \left\{ \frac{1}{4m} \left(-\frac{2e}{c} \Psi^* \delta\mathbf{A} \right) \cdot \left(-i\hbar\nabla\Psi - \frac{2e}{c} \mathbf{A}\Psi \right) \right. \\ &\quad \left. + \frac{1}{4m} \left(i\hbar\nabla\Psi^* - \frac{2e}{c} \mathbf{A}\Psi^* \right) \cdot \left(-\frac{2e}{c} \Psi \delta\mathbf{A} \right) \right. \\ &\quad \left. + \frac{1}{4\pi} (\text{curl } \mathbf{A} - \mathbf{H}_0) \cdot \text{curl } \delta\mathbf{A} \right\} dV. \end{aligned} \quad (3.13)$$

One notices that $\delta\mathbf{A}$ in (3.13) could be taken out of the brackets but for the term $(1/4\pi)(\text{curl } \mathbf{A} - \mathbf{H}_0) \cdot \text{curl } \delta\mathbf{A}$. Using the identity

$$\mathbf{a} \cdot \text{curl } \mathbf{b} = \mathbf{b} \cdot \text{curl } \mathbf{a} - \text{div}[\mathbf{a} \times \mathbf{b}], \quad (3.14)$$

Coherence length ξ

with the right coefficients: $\psi(x) = \psi_\infty \tanh(x/2^{1/2}\xi)$

with:

Coherence length ξ : $\xi^2 = \hbar^2/(m^*a(T_C - T)),$

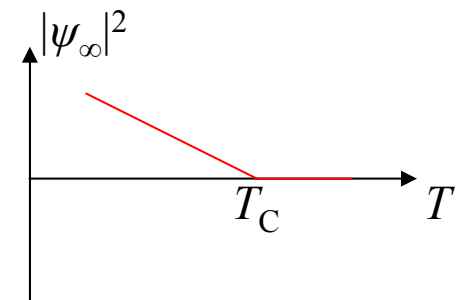
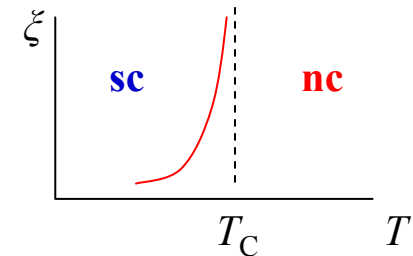
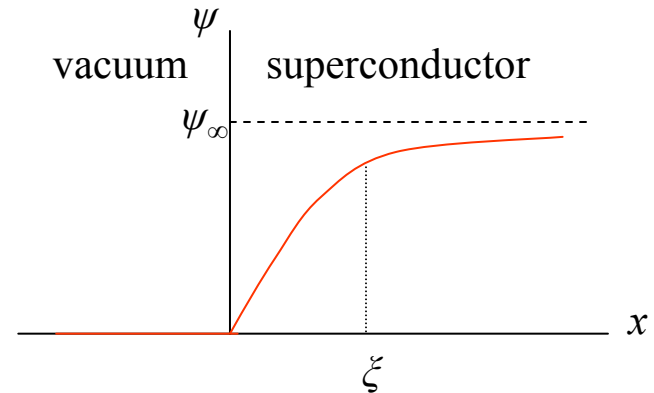
i.e. $\xi \sim (T_C - T)^{-1/2}$

diverges with critical exponent $\nu = 1/2$

and pre-factor $|\psi_\infty|^2 = a(T_C - T)/\lambda$ **below** T_C .

The coherence length ξ gives the distance over which the sc-wave function can change significantly.

The density $|\psi_\infty|^2$ of sc-electrons grows linearly with distance from the transition temperature:



London penetration depth λ_L

b) with magnetic field $\mathbf{B} \neq 0$,
and only weakly variable $\psi(x)$:

2nd Ginzburg-equation $\partial F_s / \partial \mathbf{A} = 0$

gives the spatial dependence of the field $\mathbf{B}(\mathbf{x})$:

$$\nabla^2 \mathbf{A} = \mathbf{A} / \lambda_L^2 + \psi^* \nabla \psi + \dots \quad (\text{with } \nabla^2 \mathbf{A} = (\nabla^2 A_x, \nabla^2 A_y, \nabla^2 A_z))$$

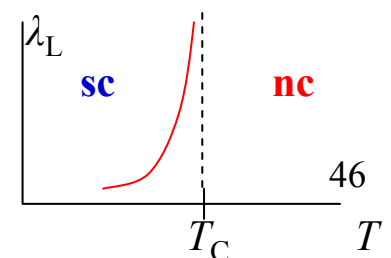
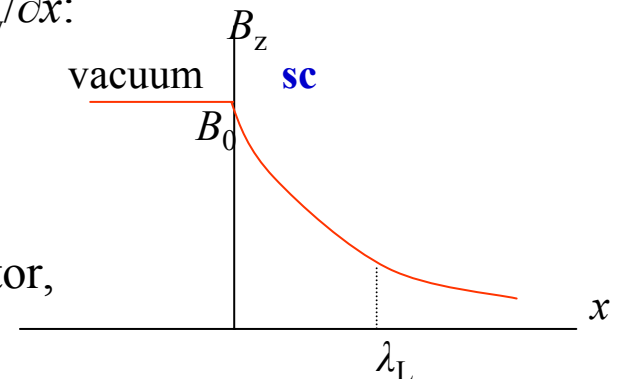
$$\uparrow \approx 0$$

With $\mathbf{B} = (0, 0, B_z)$, i.e. $\mathbf{A} = (0, A_y, 0)$, $\mathbf{x} = (x, 0, 0)$:
only $\partial^2 A_y / \partial x^2 = A_y / \lambda_L^2$ contributes, and from $B_z = \partial A_y / \partial x$:
 $\partial^2 B_z / \partial x^2 = B_z / \lambda_L^2$:

$$B_z(x) = B_0 \exp(-x / \lambda_L)$$

The magnetic field cannot penetrate into the superconductor,
but decays exponentially, which is the Meissner effect:

with London penetration depth λ_L : $\lambda_L^2 = m^* / (\mu_0 e^{*2} |\psi_\infty|^2)$,
i.e. $\lambda_L \sim (T_C - T)^{-1/2}$ diverges in the same way as coherence length ξ :



Energy balance

Meissner-effect at the critical field $B \rightarrow B_C^+$, with sudden expulsion of the magnetic field:

The energy needed to expel the field B_C from the volume V is:

$$E_{\text{mag}} = VB_C^2/2\mu_0 > 0.$$

This energy is taken from the energy gained during the transition to superconductivity:

$$E_{\text{gap}} = -E_{\text{mag}} < 0. \quad \overline{\overline{E_{\text{gap}}}} \downarrow$$

For a given λ_L , ξ , and surface A :

In the Meissner boundary layer of thickness λ_L ,
no field is expelled from the volume $\lambda_L A$:

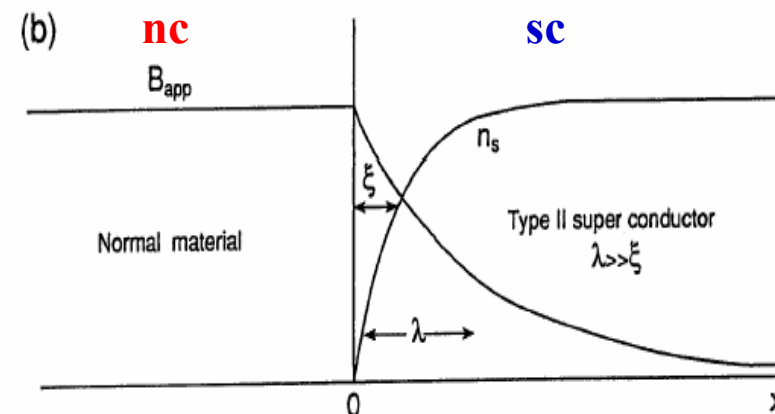
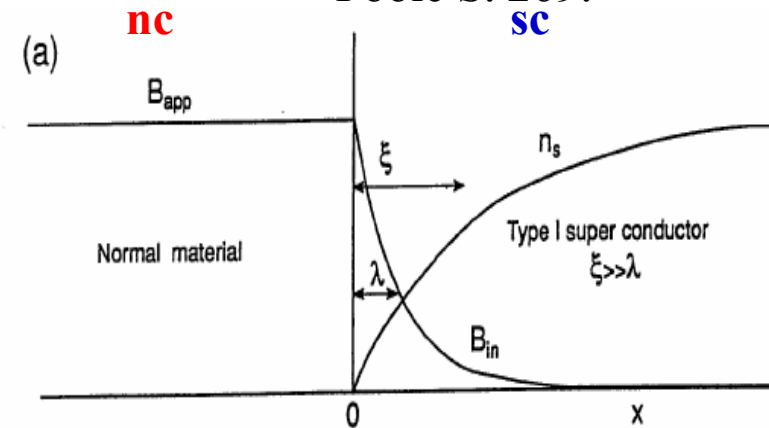
$$\Delta E_{\text{mag}} = -\lambda_L A B_C^2/2\mu_0 < 0.$$

In the coherence boundary layer of thickness ξ ,
no Cooper pairs are formed in the volume ξA :

$$\Delta E_{\text{gap}} = +\xi A B_C^2/2\mu_0 > 0.$$

Energy balance : $\Delta E = (\xi - \lambda_L)B_C^2/2\mu_0.$

Poole S. 269:
sc



Superconductor of the 1st and 2nd type

Superconductor of the 1st type has $\Delta E > 0$, i.e.:

coherence length ξ > penetration depth λ_L ,

area A is minimized to Meissner boundary layer at the surface
(true for all superconducting elements except Nb).

Superconductor of the 2nd type has $\Delta E < 0$, i.e.:

coherence length ξ < penetration depth λ_L

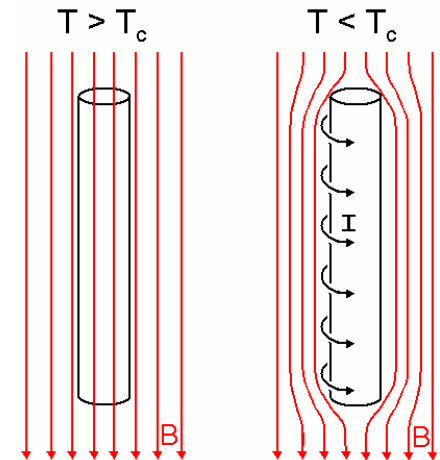
area A is maximized to many flux tubes,
(true for many superconducting compounds).

From BCS:

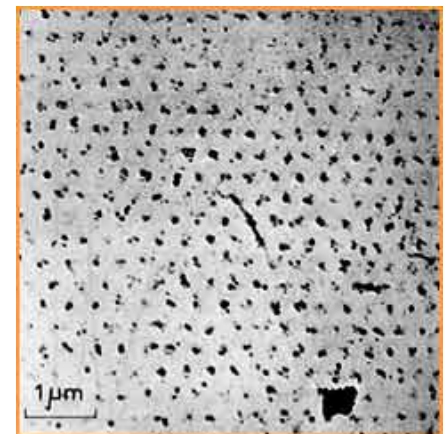
The circular currents of the Cooper pairs are quantized,
each flux tube containing exactly one flux quantum of size

$$\Phi_0 = h/2e$$

Superconductor of the 1st type:

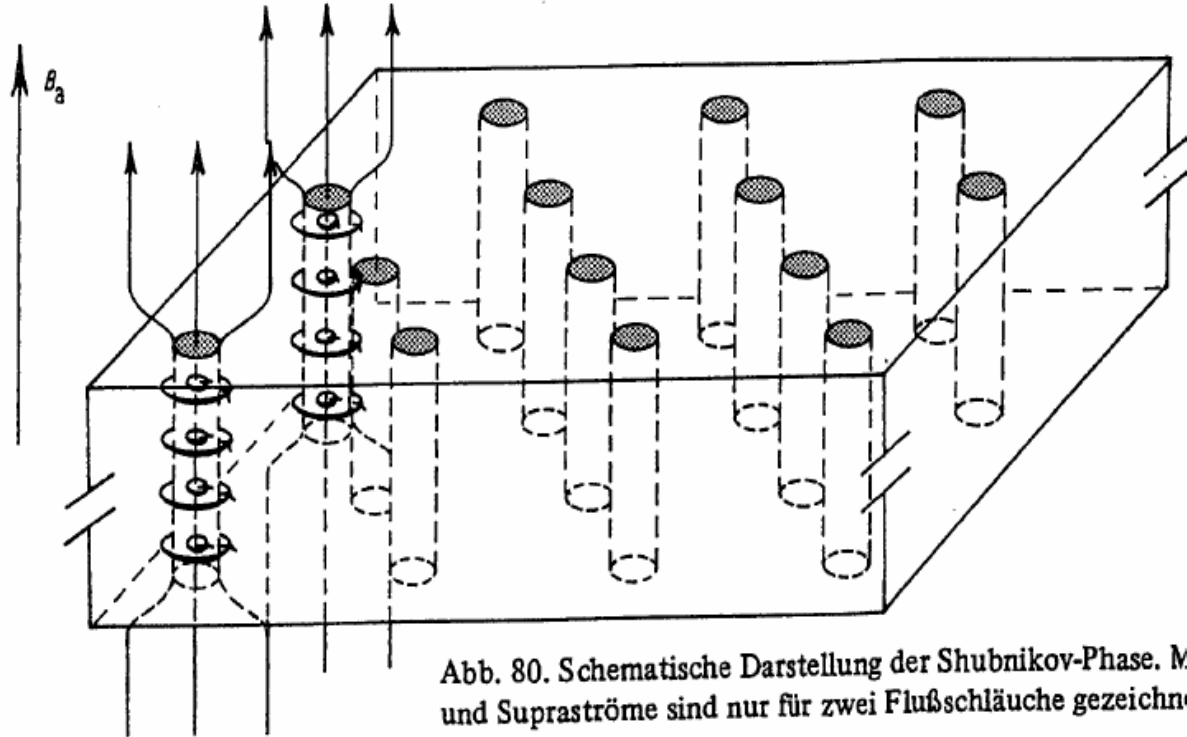


Superconductor of the 2nd type:



Flux-quantisation

Buckel Supraleitung, p. 150:



Conclusion:

Mean-field Ginzburg-Landau theory describes the main phenomena of superconductivity, **but is not a microscopic theory** like BCS.

7. Gauge invariance of electro-magnetic interaction

El.-Dyn. in covariant notation:

field-tensor:

$$F_{\mu\nu} = \begin{pmatrix} 0 & B_z & -B_y & -iE_x \\ -B_z & 0 & B_x & -iE_y \\ B_y & -B_x & 0 & -iE_z \\ iE_x & iE_y & iE_z & 0 \end{pmatrix}$$

four-vectors:

$$\partial_\mu = (\nabla, i\partial/\partial t), \quad j_\mu = (j, i\rho)$$

conventional notation:

Maxwell equations, inhomog.:

$$c^2 \nabla \times \mathbf{B} - \partial \mathbf{E} / \partial t = \mathbf{j} / \epsilon_0, \quad \nabla \cdot \mathbf{E} = \rho / \epsilon_0$$

continuity-equation:

$$\nabla \cdot \mathbf{j} + \partial \rho / \partial t = 0$$

el.-magn. potentials \mathbf{A} , Φ :

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\nabla \Phi$$

canonical momentum:

$$\mathbf{D} = \nabla - ie\mathbf{A}, \quad D_0 = \partial/\partial t + ie\Phi$$

photon is invariant against gauge transformation:

$$\mathbf{A}' = \mathbf{A} + \nabla \theta, \quad \Phi' = \Phi - (1/c)\partial\theta/\partial t$$

covariant notation:

$$\partial_\mu F_{\mu\nu} = j_\nu \quad (\text{NB: sum-convention})$$

$$\partial_\mu j_\mu = 0 \quad (= \text{conserved current})$$

$$A_\mu = (\mathbf{A}, i\Phi):$$

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

$$D_\mu = \partial_\mu - ieA_\mu$$

$$A'_\mu = A_\mu + \partial_\mu \theta$$

Gauge symmetry U(1) of QED

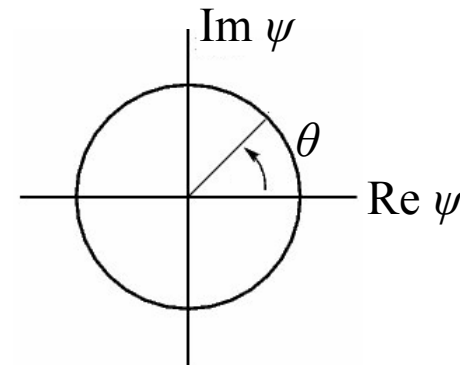
Gauge invariance = invariance against arbitrary phase shifts:

Is also electron wave function gauge invariant?

Free electron, wave function $\psi(x)$, with $x = (\mathbf{x}, it)$:

Global, arbitrary phase shift: $\psi' = \psi \exp(i\theta)$

does not change probability: $|\psi'|^2 = |\psi|^2$



But: Such a global Symmetry is not Lorentz-invariant!

Reasonable is only an arbitrary position dependent shift in phase $\theta = \theta(x)$:

$$\psi'(x) = \psi(x) \exp(i\theta(x)) \quad \text{U(1) transformation}$$

Gauge invariance = invariance against local phase shifts = local symmetry

But: If interaction is invariant against phase shifts with arbitrary $\theta(x)$:

then a wave function

$$\psi(x):$$

can be changed into anything: $\psi'(x)$:

not helpful

Gauge invariance of Dirac equation ...

Equation of motion $\psi(x)$ of free electron = Dirac equation:

$$(\gamma_\mu \partial_\mu + m) \psi = 0$$

= 4 differential eqs. for the 4 components ψ_v ,

Coefficients = 4-vectors γ_μ

whose components are matrices, for instance:

$$\gamma_3 = \begin{pmatrix} 0 & -i\sigma_z \\ i\sigma_z & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}$$

Dirac-equation alone is not gauge invariant:

Proof: Transformation $\psi'(x) = \psi(x) \exp(i e \theta(x))$

with chain rule $\partial_\mu \psi' = (\partial_\mu \psi) e^{i e \theta} + \psi i e (\partial_\mu \theta) e^{i e \theta}$

the Dirac equation changes to:

$$(\gamma_\mu \partial_\mu + m) \psi' = (\gamma_\mu \partial_\mu + m) \psi e^{i e \theta} + i e (\partial_\mu \theta) \psi e^{i e \theta} = 0 + i e (\partial_\mu \theta) \psi' \\ \uparrow \text{extra dynamics}$$

hence, after the transformation, Dirac equation no longer holds:

$$(\gamma_\mu \partial_\mu + m) \psi' \neq 0$$

... requires existence of (massless) photon ...

For Dirac equation to be gauge invariant, i.e.

for world of electrons to be invariant against arbitrary phase shifts $\theta(x)$: $\psi'(x) = \psi(x) e^{ie\theta(x)}$

necessarily the photon must exist

which is a gauge invariant vector field A_μ :

$$A'_\mu = A_\mu + \partial_\mu \theta$$

which couples to the electron (with scale factor e = "charge")

$$D_\mu \psi = (\partial_\mu - ieA_\mu) \psi$$

(and which obeys Maxwell's equations)

When in Dirac equation ∂_μ is replaced by the **covariante derivative D_μ** :
then the Dirac equation becomes gauge invariant:

$$\begin{aligned} D'_\mu \psi' &= (\partial_\mu - ieA'_\mu) \psi e^{ie\theta} = \partial_\mu (\psi e^{ie\theta}) - ie(A_\mu + \partial_\mu \theta) \psi e^{ie\theta} \\ &= (\partial_\mu \psi) e^{ie\theta} + ie(\partial_\mu \theta) \psi e^{ie\theta} - ieA_\mu \psi e^{ie\theta} - ie(\partial_\mu \theta) \psi e^{ie\theta} \\ &= e^{ie\theta} (\partial_\mu - ieA_\mu) \psi = e^{ie\theta} D_\mu \psi \end{aligned}$$

that is with:
holds.

$$\boxed{(\gamma_\mu D_\mu + m) \psi = 0} \quad \text{also:} \quad \boxed{(\gamma_\mu D'_\mu + m) \psi' = e^{ie\theta} (\gamma_\mu D_\mu + m) \psi = e^{ie\theta} \cdot 0 = 0}$$

Conclusion: Free electrons cannot exist alone, but only together with photons.

... and the conservation of electric charge

Electron in an external potential A : $\psi = \psi_0 \exp(i(p - eA)x)$,

A change in potential energy by $e\Delta A$ induces phase shift $\exp(ie\Delta A \cdot x)$,

i.e. gauge symmetry, the free choice of local phase, means free choice of local zero of energy

gauge symmetry \leftrightarrow conservation of charge:

'Proof' (E. Wigner, quoted in D.H. Perkins: Elementary particle physics, ch. 3.6.1):

Assume the contrary: gauge symmetry exists without charge conservation,
but energy conservation holds:

No charge conserv.: charge e is created in an electrostatic potential Φ , i.e. $A = (0, i\Phi)$,
with energy cost W ;
charge e moves to another location with potential $\Phi' \neq \Phi$,
with energy cost $e(\Phi - \Phi') \neq 0$,
and disappears with energy gain W' .

Gauge symmetry: W is independent of $e\Phi$ (which determines phase), i.e. $W' = -W$.

Energy balance: $W - W + e(\Phi - \Phi') \neq 0$ in contradiction to energy conservation

Noether's theorem

This follows also from Noether's theorem:

Continuous symmetry \leftrightarrow conservation law

Further 'trivial' examples:

1. time shift symmetry \leftrightarrow energy conservation:

Proof: Dynamics of a system described by Hamiltonian

does not change under an arbitrary time shift dt :

if and only if $\partial H / \partial t = 0$,

i.e. if and only if energy is conserved:

$$H = T + V = E$$

$$dH = (\partial H / \partial t) dt = 0$$

$$E = \text{const.}$$

2. position shift symmetry \leftrightarrow momentum conservation:

Proof: Dynamics does not change under a shift of position $d\mathbf{x}$: $dH = \nabla H \cdot d\mathbf{x} = 0$

if and only if $\nabla H = 0$,

i.e. if and only if $d\mathbf{p}/dt = -\nabla V = -\nabla H = 0$:

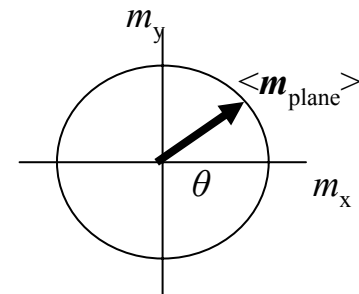
$$\mathbf{p} = \text{const.}$$

using Newton's law with $H = \mathbf{p}^2/2m + V(\mathbf{x})$

8. Higgs mechanism in a superconductor

Goldstone's theorem:

Each spontaneous breaking of a continuous symmetry
creates a massless particle (i.e. an excitation without an energy gap)
 = Goldstone Boson



Simple example: Landau ferromagnet

Free energy density f , magnetization density \mathbf{m} ,
 isotropic interaction in 3-dim:

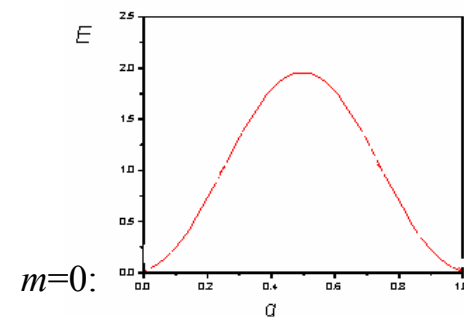
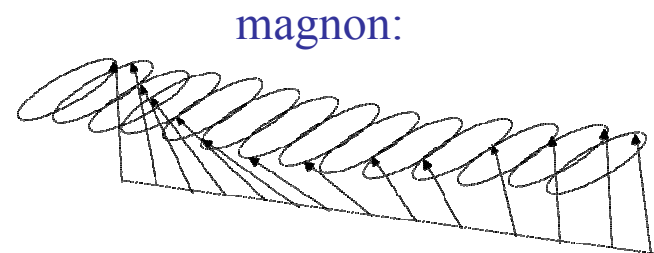
$$f = f_0 + \frac{1}{2}a \cdot (T - T_C) |\mathbf{m}|^2 + \frac{1}{4}\lambda |\mathbf{m}|^4$$

solution **above** T_C is rotationally symmetric: 

solution **below** T_C is cylindrically symmetric: 

Goldstone mode belonging to broken symmetry = **magnon**

magnon dispersion relation:



Goldstone theorem

Example superconductor in zero field, Ginzburg-Landau:

Lagrange density $L = E_{\text{kin}} - V$, complex s.c. electron $\psi = \psi_1 + i\psi_2$:

$$L_s = L_n + |\nabla\psi|^2 - \frac{1}{2}\mu^2|\psi|^2 - \frac{1}{4}\lambda'|\psi|^4$$

(rescaled, with $\mu^2 = 2m^*a \cdot (T - T_C)$, $\lambda' = 2m^*\lambda$, $\hbar = c = 1$)

below T_C : spontaneous breaking of symmetry,

with fluctuations of amplitude ψ and phase θ about mean $\langle\psi\rangle = (a \cdot (T - T_C)/\lambda)^{1/2} \equiv v$:

$$\psi(x) = (v + \chi(x)) \exp(i\theta(x)/v)$$

With $x=(x, it)$. For small fluctuations $\chi \ll v$,

using $|\nabla\psi|^2 = |\nabla\chi + i(v + \chi) \nabla\theta/v|^2 \approx (\nabla\chi)^2 + (\nabla\theta)^2$ etc.

inserted into L_s this leads to:

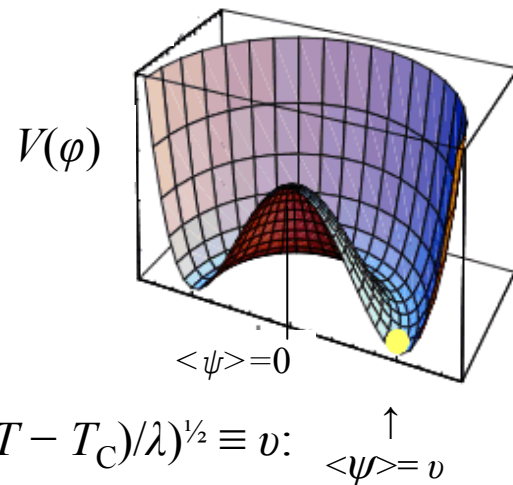
$$L_s = \text{const.} + (\nabla\chi)^2 - \frac{1}{2}\mu^2 \chi^2 = \text{excitation } \chi \text{ of mass } \mu$$

$$+ (\nabla\theta)^2 = \text{appearance of Goldstone } \theta \text{ without mass term}$$

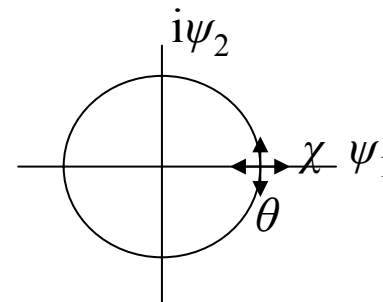
$$+ \dots = \text{higher order interactions neglected}$$

(at the minimum, linear term $-\mu^2 v \chi$ disappears)

(Lagrange density L and its mass terms μ to be discussed later),



seen from above:



Higgs-mechanism in superconductor

Gauge invariance requires interaction with massless field A_μ .

However, in a superconductor, the photon A_μ becomes massive.

Still: Ginzburg-Landau model is gauge invariant (Dr.-thesis Ginzburg ~ 1950)

The reason is what is now called the Higgs mechanism:

When a scalar, gauge invariant field ψ
suffers a spontaneous symmetry breaking,
then the vectorfield A_μ can become massive,
without losing its gauge invariance,
while at the same time the Goldstone disappears.

Ginzburg-Landau superconductor of Ch. 6:

Cooper pairs = Higgs field ψ :

$$L_s = L_n + |\nabla\psi - i2e\mathbf{A}\psi|^2 - \frac{1}{2}\mu^2|\psi|^2 - \frac{1}{4}\lambda'|\psi|^4 - \mathbf{B}^2/\mu_0^* + \mathbf{B}\cdot\mathbf{M}$$

with charge of Cooper pairs $e^* = 2e$.

Disappearance of the Goldstone boson

As before: Fluctuations of $\psi(x)$ about $\langle\psi\rangle = v$ at "bottom of bottle"

$$\psi(x) = (v + \chi(x)) \exp(i\theta(x)/v)$$

Then $|\nabla\psi - ie^*A\psi|^2 = |\nabla\chi + i(v + \chi)(\nabla\theta/v - e^*A)|^2$, with $\chi \ll v$:

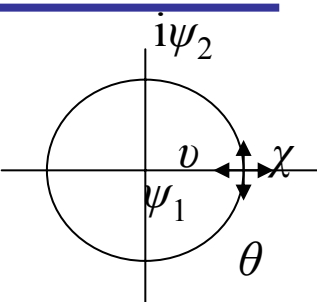
if we choose gauge to $A=A' + \nabla\theta/e^*v$, this becomes $\approx (\nabla\chi)^2 - v^2e^{*2}A'^2$,

and the massless Goldstone term $(\nabla\theta)^2$ disappears,

and the photon A becomes massive (but remains gauge invariant):

$$\begin{aligned} L_s = \text{const.} + (\hbar^2/2m^*) (\nabla\chi)^2 - \frac{1}{2}\mu^2|\chi|^2 &= \text{"Higgs" with mass } \mu \\ -m_{\text{ph}}^2A'^2 &= \text{heavy photon with mass } m_{\text{ph}} = ve^* = (a \cdot (T - T_C)/\lambda)^{1/2} 2e \\ -\mathbf{B}^2/2\mu_0 + \mathbf{B} \cdot \mathbf{M} &= \text{field terms as before} \\ &+ \text{some residual terms} \end{aligned}$$

The coherence length found before turns out to be $\xi = 1/\mu$ ($\hbar = c = 1$),
 or $\xi = \hbar/\mu c = \text{Compton wave length of the Higgs of mass } \mu = (4ma \cdot (T_C - T))^{1/2}$,
 and the London penetration depth $\lambda_L = 1/m_{\text{ph}}$, or $\lambda_L = \hbar/m_{\text{ph}}c$
 = Compton wave length of the heavy photon



N.B.: number of degrees of freedom remains the same

Summary superconductivity

Mean field theory of superconductivity (Ginzburg-Landau):

Phase transition at transition temperature T_C = spontaneous symmetry breaking

Superconductor has 2 characteristic scales:

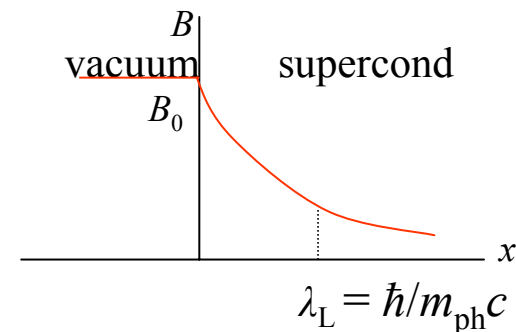
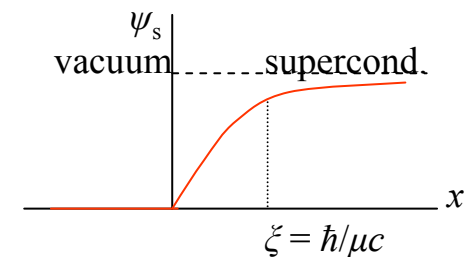
1. of the order parameter = superconducting condensate ψ ,
whose fluctuations lead to the Higgs field χ of mass μ
whose Compton wavelength $\hbar/\mu c$
= coherence length ξ of the condensate.

2. of the magnetic field, via the Meissner effect:

The field-producing virtual photons become massive,
with mass $m_{\text{ph}} = e^* v = e^* \langle \phi \rangle$

Hence the magnetic field B has only a limited range given by
the Compton wavelength $\hbar/m_{\text{ph}} c$ of the massive photon
= London penetration depth λ_L

but no Goldstone survives. The theory remains gauge invariant.



8. Electroweak unification

Preliminaries, Lit.: U. Mosel, Fields, Symmetries, and Quarks, Springer, 1989, Ch. 3.

Lagrange: $L = T - V = L(x, \dot{x})$

Euler \rightarrow equ's of motion: $\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0$

examples:

1. harmonic oscillator: $L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2$

Euler \rightarrow **oscillation eq.** $\frac{d}{dt} m \dot{x} + kx = m \ddot{x} + kx = 0$

2. scalar field ϕ (Spin - 0 Boson wie π)

relativist. total energy $E^2 = \mathbf{p}^2 + m^2 \quad (c = 1)$

with $p = p_\mu = (\mathbf{p}, iE)$: $p^2 = \mathbf{p}^2 - E^2 = -m^2$, oder $p^2 + m^2 = 0$,

i.e., with $i\partial_\mu = p_\mu = (\mathbf{p}, iE)$:

Klein - Gordon equation: $\partial_\mu^2 \phi - m^2 \phi = 0$

has Lagrange - density: $L = -\frac{1}{2} ((\partial_\mu \phi)^2 + m^2 \phi^2)$

Check: Variation in ϕ : $\partial_\mu \frac{\partial L}{\partial (\partial_\mu \phi)} - \frac{\partial L}{\partial \phi} = 0$

gives Klein - Gordon eq.: $\partial_\mu (-\partial_\mu \phi) + m^2 \phi = 0$ O.K.

Preliminaries cont'd

3. Spinor field ψ (spin -1/2 fermions: e, q, ...)

Lagrange: $L = -\bar{\psi}(\gamma_\mu \partial_\mu + m)\psi$ mit $\bar{\psi} = \psi^\text{T} \gamma_4$

Euler \rightarrow **Dirac**: $\partial_\mu(-\bar{\psi}\gamma_\mu) + m\bar{\psi} = (\gamma_\mu \partial_\mu + m)\psi = 0$

conserved current: $j_\mu = -e\bar{\psi}\gamma_\mu\psi$

4. Massless vector field A_μ (spin -1 photon γ , 2 degrees of freedom $M = \pm 1$)

Lagrange: $L = -1/4 F_{\mu\nu} F_{\mu\nu}$ (mit $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$)

is gauge invariant: $F_{\mu\nu}' = \partial_\mu A_\nu' - \partial_\nu A_\mu' = \partial_\mu(A_\nu + \partial_\nu \theta) - \partial_\nu(A_\mu + \partial_\mu \theta) = F_{\mu\nu}$

Euler \rightarrow **electro - magnetic waves.**

5. Coupling to charges: $L = -1/4 F_{\mu\nu} F_{\mu\nu} + j_\mu A_\mu$

Euler \rightarrow **Maxwell Glg.**

6. QED: $L = -1/4 F_{\mu\nu} F_{\mu\nu} + \bar{\psi}(\gamma_\mu \partial_\mu + m)\psi - e\bar{\psi}\gamma_\mu\psi A_\mu$, electron - mass m

$\uparrow j_\mu A_\mu$

7. Massive vector field A_μ (spin -1 W, Z - bosons, supercond.: 3 d.o.f. $M = 0, \pm 1$)

Lagrange: $L = -1/4 F_{\mu\nu} F_{\mu\nu} - 1/2 m^2 A_\mu A_\mu$, boson mass m

is **not gauge - invariant**, exsept via Higgs Mechanism

Electro-magnetic vs. weak interactions

Differences between el.-magn. and weak interactions (numbers for $E=0$):

Problem	El.-magn. interact	Weak interaction	solution of problem
Strength of interaction	$\alpha = 1/137$	10^{-5}	Higgs-mechanism
Range of interaction	∞	$\lambda_C(W) \sim 10^{-16} \text{ cm}$	
\rightarrow Mass int. particle	$m_\gamma = 0$	$m_W \sim 90 \text{ GeV}$	
gauge invariance	yes	no	
Parity conservation	yes	no	$j_\mu = \psi' \gamma_\mu (1 - \gamma_5) \psi$
Renormalizability	yes	no	t'Hooft

Standard Model: the particles

$SU(2) \times U(1)$:

The basic particles :

Fermions : L - handed doublets $\psi_L = \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} = \begin{pmatrix} (1 - \gamma_5) \psi_\nu / 2 \\ (1 - \gamma_5) \psi_e / 2 \end{pmatrix}$

 R - handed singlets $\psi_R = (e_R) = ((1 + \gamma_5) \psi_e / 2)$

Higgs - scalar : Doublet $\phi = \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix}$

Field tensors etc. in QED and in Standard Model

QED U(1):

Field tensor: $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$

covariant derivative: $D_\mu = \partial_\mu - ieA_\mu$

Standard model SU(2)×U(1):

Field tensors: $W_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu - gA_\mu \times A_\nu$
 $B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$

SU(2) \times U(1) gauge transformations

Gauge transformation simultaneously for :

$$\begin{aligned}\text{SU}(2): \quad \psi_L' &= \psi_L \exp(-ig\boldsymbol{\alpha} \cdot \boldsymbol{\tau} / 2) \\ \psi_R' &= \psi_R\end{aligned}$$

$$\begin{aligned}\text{U}(1): \quad \psi_L' &= \psi_L \exp(-iY_L\theta / 2) \\ \psi_R' &= \psi_R \exp(-iY_R\theta / 2)\end{aligned}$$

with weak isospin $\boldsymbol{\tau}$

and weak hypercharge $Y = 2(Q - \tau_3)$

e.g. $Y_L = -1$ für e_L^- und ν_e , $Y_L = -2$ für e_R^-

covariant derivative :

$$\text{for doublet } \psi_L : \quad D_\mu = \partial_\mu + ig\boldsymbol{A}_\mu \cdot \boldsymbol{\tau} / 2 - ig'B_\mu$$

$$\text{for singlet } \psi_R : \quad d_\mu = \partial_\mu - 2ig'B_\mu$$

with gauge bosons :

$$\boldsymbol{A}_\mu' = \boldsymbol{A}_\mu + \partial_\mu \boldsymbol{\alpha} + g(\boldsymbol{\alpha} \times \boldsymbol{A}_\mu)$$

and

$$B_\mu' = B_\mu + \partial_\mu \theta \quad (\text{like el. - dyn.})$$

Lagrangian of QED and of Standard Model

cf. QED U(1):

$$\begin{aligned} L = & -(1/4)F_{\mu\nu}F_{\mu\nu} & (\text{Gauge boson} = \text{photon } \gamma) \\ & + \bar{\psi}(\gamma_{\mu}D_{\mu} + m)\psi & (\text{Fermion} = e^{-}) \\ & - e\bar{\psi}\gamma_{\mu}\psi A_{\mu} & (\text{Interaction } e^{-} - \gamma) \end{aligned}$$

electroweak interaction SU(2)×U(1):

$$\begin{aligned} L = & -(1/4)W_{\mu\nu}W_{\mu\nu} - (1/4)B_{\mu\nu}B_{\mu\nu} & (\text{Gauge boson } W^{\pm}, Z^0, \gamma) \\ & + \bar{\psi}_L(\gamma_{\mu}D_{\mu} + m)\psi_L + \bar{\psi}_R(\gamma_{\mu}d_{\mu} + m)\psi_R & (\text{Fermions } e_L, \nu_e, e_R) \\ & - e\bar{\psi}\gamma_{\mu}\psi A_{\mu} & (\text{Electron - photon interaction}) \\ & + (1/2)D_{\mu}^2\phi + \mu^2\phi^2 + (1/4)\lambda\phi^4 & (+ \text{ terms à la Ginzburg - Landau}) \end{aligned}$$

Summary: non-Abelian gauge theories

Symmetry	Symm. group	U(1)	SU(2)	SU(3)
	Type	Abelian	non-Abelian (Yang-Mills)	
	Example	QED	isospin (strong, weak)	flavour, colour QCD
	Multiplet	(e); (p) ...	(p,n); (u,d); (e,v _e) ...	(u,d,s); (r,b,g) ...
Gauge trans-form.	Particle	$\varphi' = \varphi \exp(i e \theta(x))$	$\varphi' = \varphi \exp(i g \boldsymbol{\alpha}(x) \cdot \boldsymbol{\tau} / 2)$	$\varphi' = \varphi \exp(i g_s \alpha_i(x) \cdot \lambda_i)$
	"Generator"	1	3 Pauli matrices $\boldsymbol{\tau}$	8 Gell-Mann matr. λ_i
	Int.-boson $m=0$	$\gamma: A' = A_\mu + \partial_\mu \theta$	$A'_\mu = A_\mu - \partial_\mu \boldsymbol{\alpha} - g \boldsymbol{\alpha} \times A_\mu$	gluons $G'_{\mu i} = G_{\mu i} - \partial_\mu \alpha_i - g_s f_{ijk} \alpha_j G_{\mu k}$
	Covariant derivative	$D_\mu = \partial_\mu - i e A_\mu$	$D_\mu = \partial_\mu + i g \boldsymbol{\tau} \cdot A_\mu / 2$	$D_\mu = \partial_\mu + i g_s \lambda_i \cdot G_{\mu i} / 2$
	Indices	$\mu=1, \dots, 4$ for x, y, z, it	$A_\mu = (A_\mu^1, A_\mu^2, A_\mu^3)$	$i = 1, \dots, 8$

e.g. SU(2): $\boldsymbol{\tau} \cdot A_\mu = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} A_\mu^1 + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} A_\mu^2 + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} A_\mu^3 = \begin{pmatrix} A_\mu^0 & A_\mu^- \\ A_\mu^+ & -A_\mu^0 \end{pmatrix}, \quad \mu = 1, \dots, 4$

$$A_\mu^\pm = A_\mu^1 \pm i A_\mu^2$$

$$A_\mu^0 = A_\mu^3$$

Standard model

Fix gauge such that Higgs $\varphi = (0, \varphi(x))$

Fluctuations about new minimum $\varphi(x) = [v + \chi(x)] e^{i\theta(x)/v}$ as before:

Goldstone disappears, gauge fields W^\pm , Z^0 become massive, γ remains massless

Free energy superconductivity vs. standard model

Ginzburg-Landau:

$$L = | -i\hbar\nabla\psi - 2ieA\psi |^2 - \frac{1}{2}\mu^2 |\psi|^2 - \frac{1}{4}\lambda' |\psi|^4 + B^2/2\mu_0 - \mathbf{B}\cdot\mathbf{M} \dots$$

Weinberg-Salam:

$$L = (D_\mu\phi)^\dagger (D_\mu\phi) - \frac{1}{2}\mu^2 (\phi^\dagger\phi) - \frac{1}{4}\lambda (\phi^\dagger\phi)^2 - \frac{1}{4} W_{\mu\nu} W_{\mu\nu} - \frac{1}{4} B_{\mu\nu} B_{\mu\nu} \\ + \text{lepton and quark kinetic energies} + \dots$$

Comparison of coefficients gives:

Summary

	<u>G.-L.:</u> $U_{\text{el-mag}}(1)$	<u>W.-S.:</u> $SU_L(2) \times U_Y(1)$
<u>order parameter:</u>	super-conducting condensate $\psi = \psi_1 + i\psi_2$	Higgs doublet $\psi = (\psi_1 + i\psi_2, \psi_3 + i\psi_4)$
<u>boson mass generation by Higgs field:</u>	Meissner effect $m_{\text{ph}} = e \langle \psi_1 \rangle$	Higgs mechanism $m_W = g \langle \psi_3 \rangle$
<u>Compton wavelength λ of interacting boson:</u>	London penetration depth $\lambda_L = \hbar/(m_{\text{ph}}c)$	range of weak interaction $\lambda_W = \hbar/(m_Wc)$
<u>Compton wavelength λ of Higgs:</u>	coherence length $\xi = \hbar/(\mu c)$	"coherence length" $\lambda_H = \hbar/(m_Hc)$

10. Fluctuations near a phase transitions

Critical opalescence:

Light scattering off density variations
near the critical point of a liquid (freon).

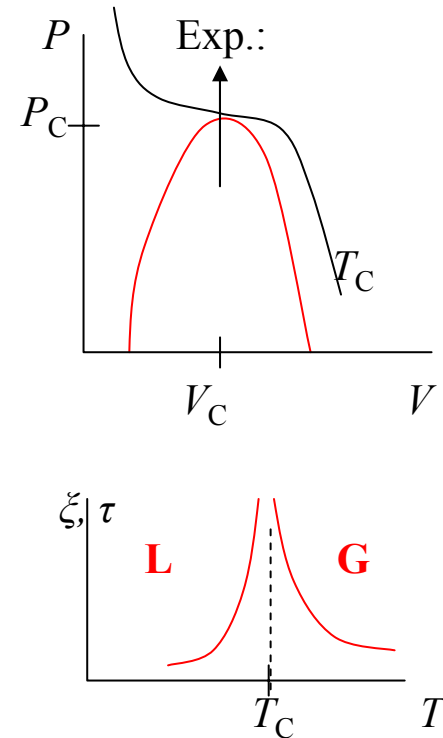
Correlation length $\xi \sim$ mean size of a region of same density

Correlation time $\tau \sim$ mean time of existence of such a region

When wavelength of light $\lambda \sim$ correlation length ξ :
strong light scattering, transmission goes to zero.

When $T \rightarrow T_C$, then density fluctuations
on all length scales and all time scales:

Divergence: $\xi \rightarrow \infty$, $\tau \rightarrow \infty$



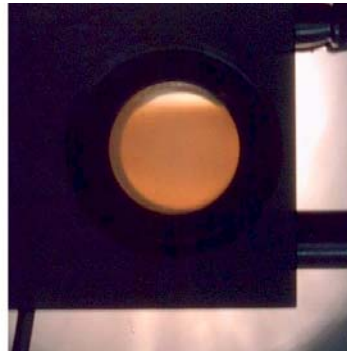
Experiment on critical opalescenc



well below T_C :
two phases



below T_C



near T_C



above T_C :
single phase

Movies:

http://www.physics.brocku.ca/courses/1p23/Heat/Critical_Point_of_Benzene/BENZENE3.MOV

<http://groups.physics.umn.edu/demo/thermo/4C5020.html>

Space-time correlations

Fluctuations are described by 'correlation functions', which tell us, how much the fluctuations are 'in phase' with each other.

The probability, to find particle at time t_i at position \mathbf{x}_i , and at a later time t_j at position \mathbf{x}_j , is given by the space-time correlation function.

Example: density correlation function:

Abbreviation: particle number density $n_i \equiv n(\mathbf{x}_i, t_i)$, with time average $\langle n_i \rangle$:

With $n_i - \langle n_i \rangle =$ fluctuations about this average value,

the pair-correlation function is

$$G_{ij} \equiv G(\mathbf{x}_i, \mathbf{x}_j, t_i, t_j) = \langle (n_i - \langle n_i \rangle) (n_j - \langle n_j \rangle) \rangle$$

or
$$G_{ij} = \langle n_i n_j \rangle - \langle n_i \rangle \langle n_j \rangle$$

in particular: $G_{ij} = 0$ for uncorrelated fluctuations $\langle n_i n_j \rangle = \langle n_i \rangle \langle n_j \rangle$

i.e. when the joint probability = product of the single probabilities.

Similarly for spin-spin correlation functions.

Measurement of the correlation-function $G(\mathbf{x}, t)$

In a homogeneous system: $G_{ij} = G(\mathbf{x}_i, \mathbf{x}_j, t_i, t_j) = G(\mathbf{x}_i - \mathbf{x}_j, t_i - t_j)$.

In a liquid or gas in the average all points (\mathbf{x}_i, t_i) are equivalent, and $G = G(\mathbf{x}, t)$.

Measurement by inelastic neutron scattering:

Energy transfer onto the neutron

for instance by a phonon in the probe:

$$E - E' = \hbar^2(k^2 - k'^2)/2m = \pm \text{phonon energy } \hbar\omega$$

Momentum transfer onto the neutron:

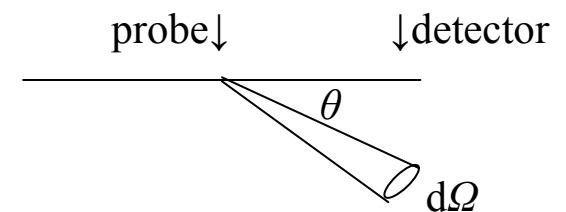
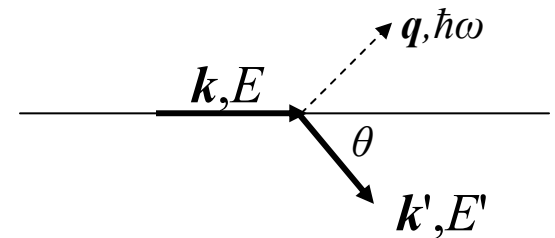
$$\mathbf{q} = \mathbf{k} - \mathbf{k}' = (\text{reciprocal lattice vector}) \pm \text{phonon momentum}$$

Differential inelastic scattering cross section:

$$d^2\sigma/d\Omega dE = \sigma_0 S(\mathbf{q}, \omega)$$

Result from scattering theory:

The scattering function $S(\mathbf{q}, \omega)$ is the space-time Fourier transform of the correlation function $G(\mathbf{x}, t)$.



Scattering functions and spatial correlations

$S(\mathbf{q}, \omega) = \text{F.T. of } G(\mathbf{x}, t)$ is very general result:

real space:

momentum space:

Solid:

Far range order

density distrib. of atoms:

Bragg peaks:

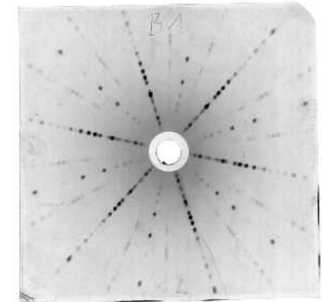
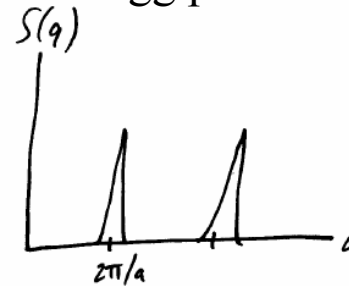
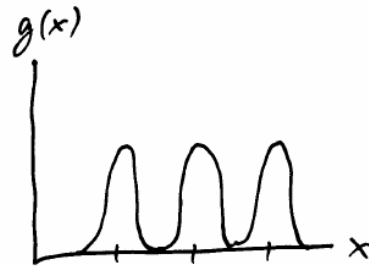


Image $S(\mathbf{q})$ of reciprocal lattice

Liquid:

Short range order

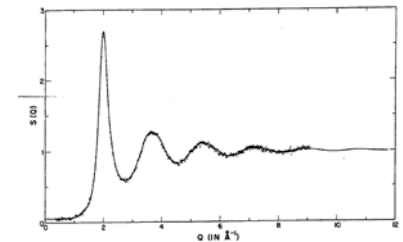
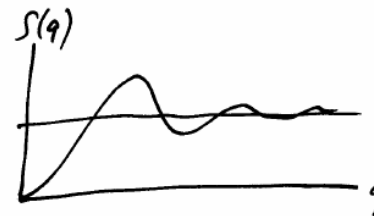
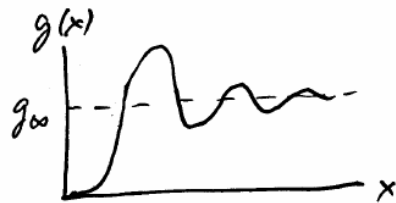
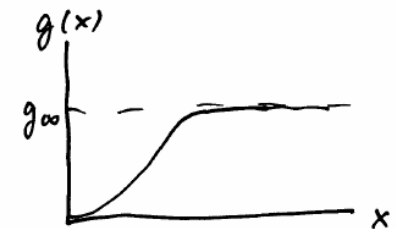


FIG. 9. Structure factor for liquid argon. [From J. L. Yarnell, M. J. Katz, R. G. Wenzel, and S. H. Koenig, *Phys. Rev. A* 7, 2130 (1973).]

Gas:

Disorder

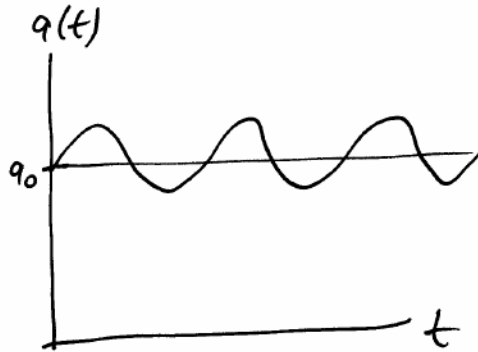


$S(q)$ of liquid argon

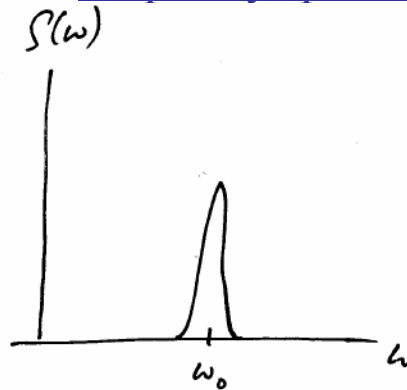
Scattering functions and time correlations

time signal

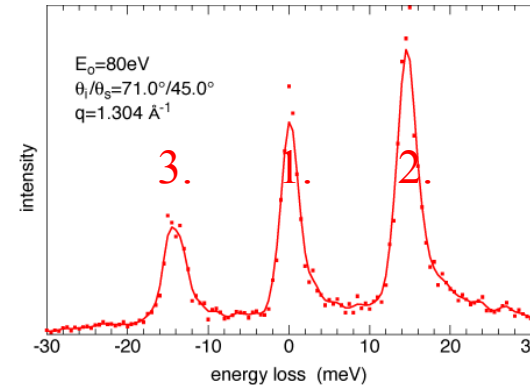
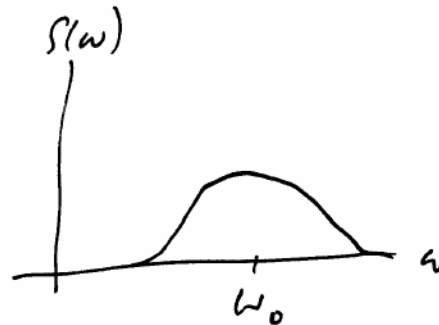
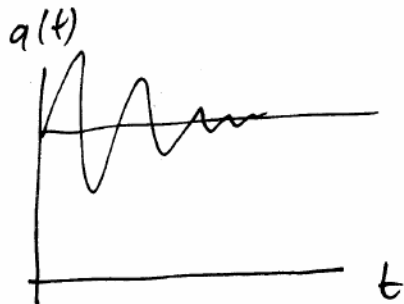
longlived:



frequency spectrum

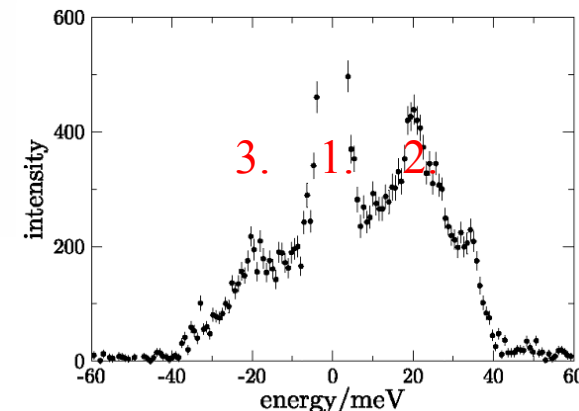


damped:



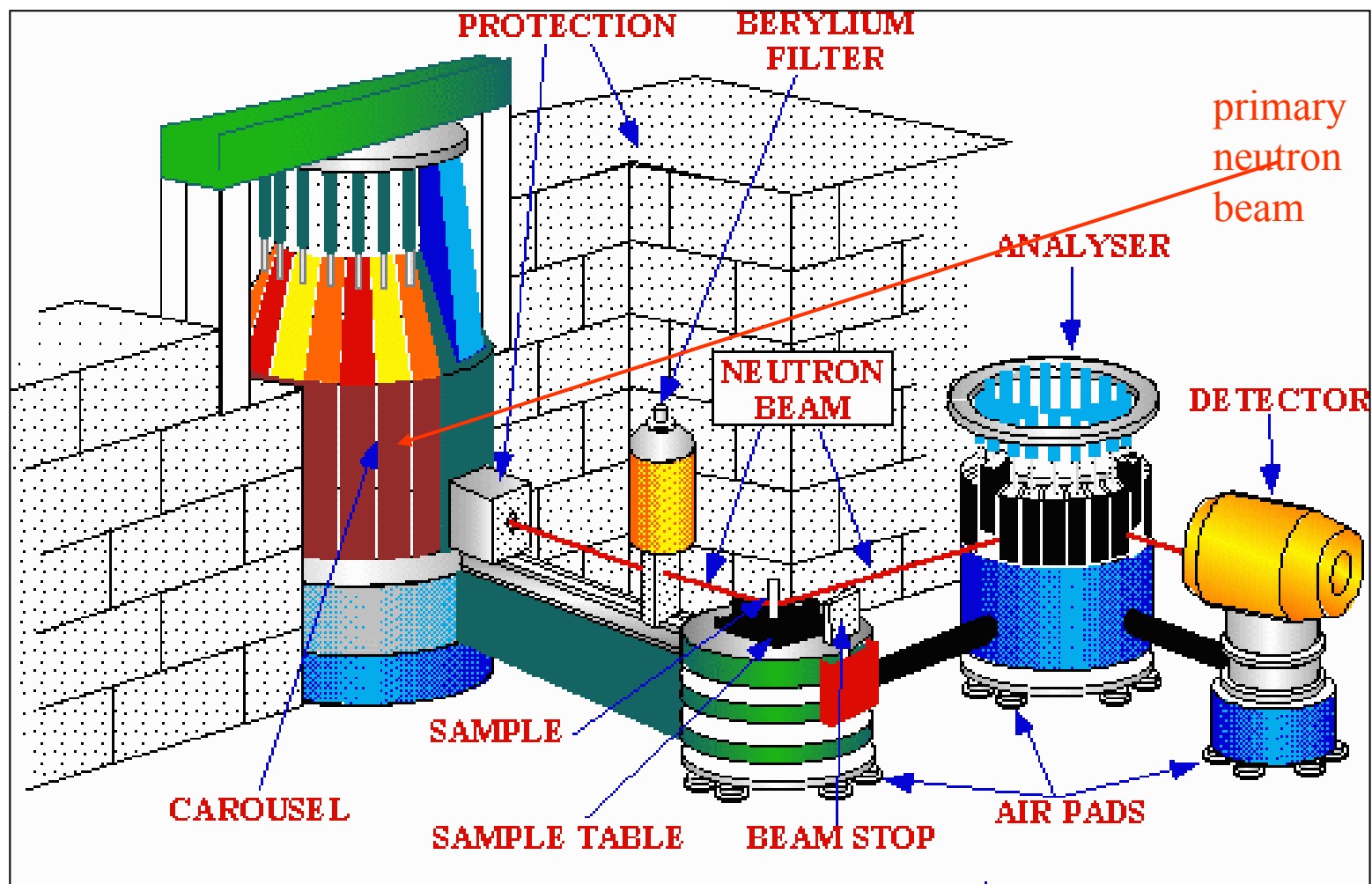
EELS spectrum from Mg(0001):

- 1. elastic peak,
- 2. creating a phonon,
- 3. destroying a phonon



Phonon spectrum of Fe islands on W(110)

Neutron three-axes spectrometer



Critical fluctuations

Fluctuations are intimately linked to the susceptibilities (proof next page):

In a liquid: density fluctuations

$$\langle \rho^2 \rangle - \langle \rho \rangle^2 = kT \cdot \kappa, \quad \text{with compressibility } \kappa.$$

In a magnet: mean square fluctuations of magnetization:

$$\langle \mathbf{M}^2 \rangle - \langle \mathbf{M} \rangle^2 = kT \cdot \chi, \quad \text{with magnetic susceptibility } \chi.$$

In particular:

At the Curie temperature: $T=T_C$ the critical magnetic fluctuations

$\langle \mathbf{M}^2 \rangle - \langle \mathbf{M} \rangle^2$ diverge like the (static) susceptibility χ ,

i.e. closely **above** T_C : $\langle \mathbf{M}^2 \rangle - \langle \mathbf{M} \rangle^2 \sim (T-T_C)^{-1}$

and closely **below** T_C half of this, because of $\chi^-(T) = \frac{1}{2} \chi^+(T)$.

N.B.: This result is closely related to the dissipation-fluctuation theorem:

The susceptibility in general is complex, its real part giving dispersion, its imaginary part giving absorption, i.e. dissipation of energy.

In electronics this is known as the Nyquist theorem:

$$\text{noise spectrum } V(\omega) = 4kT \cdot \text{resistivity } R(\omega).$$

Proof of: fluctuations \sim susceptibility

Reminder:

Mean value of an observable M :

$$\langle M \rangle = \sum_r M e^{-\beta E_r} / \sum_r e^{-\beta E_r} = \sum_r M e^{-\beta E_r} / Z$$

with partition function $Z = \sum_r e^{-\beta E_r}$

Proof of: $\langle M^2 \rangle - \langle M \rangle^2 = kT \cdot \chi$
LHS = RHS

RHS: $\chi = \partial M / \partial H = -\partial^2 F / \partial H^2 = kT \partial^2 (\ln Z) / \partial H^2$
 $= Z^{-1} \partial^2 Z / \partial H^2 - Z^{-2} (\partial Z / \partial H)^2$

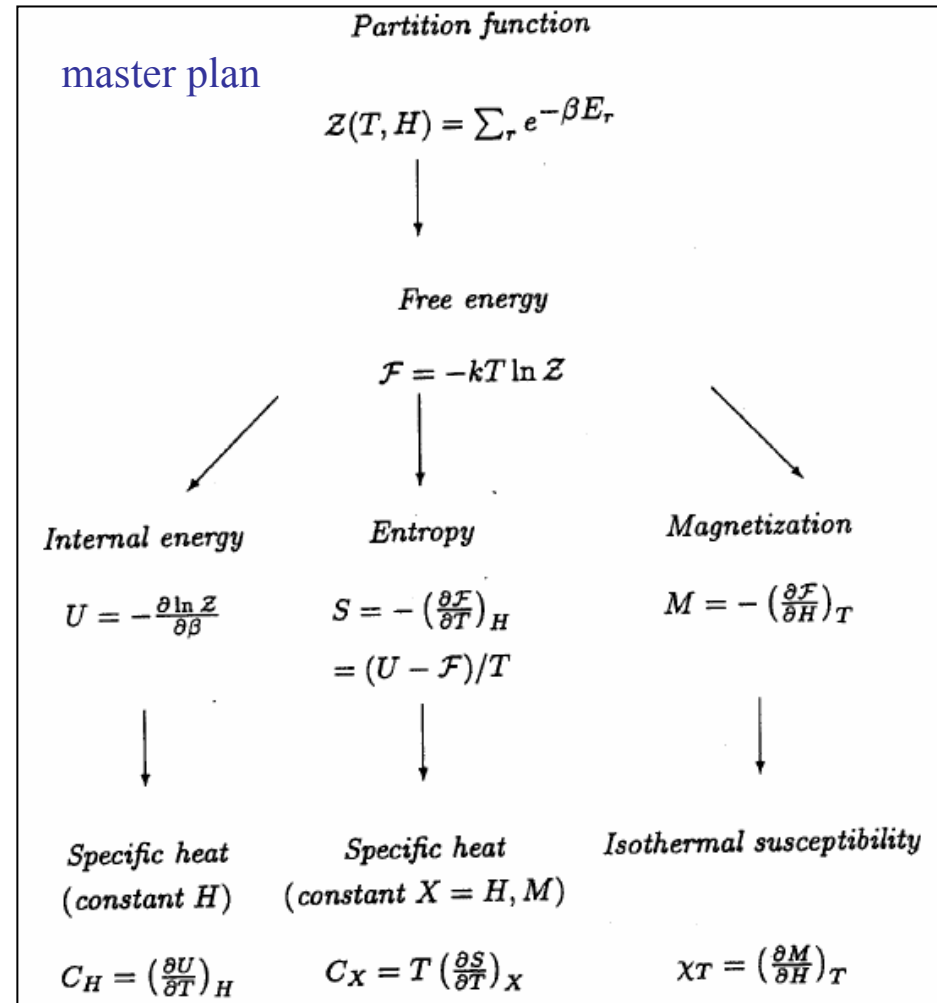
LHS: $\langle M^2 \rangle - \langle M \rangle^2$, and $E_{\text{mag}} = -M \cdot H$:

$$\langle M \rangle \equiv \sum_r M e^{-E_r/kT} / Z$$

$$= \sum_r (\partial E_r / \partial H) e^{-E_r/kT} / Z = -Z^{-1} \partial Z / \partial H$$

$$\langle M^2 \rangle \equiv \sum_r M^2 e^{-E_r/kT} / Z = Z^{-1} (\partial^2 Z / \partial H^2)$$

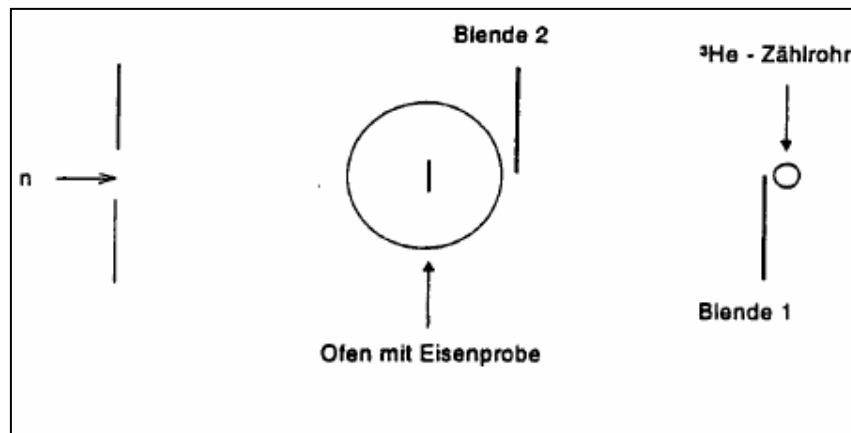
\rightarrow RHS = LHS



Measurement of magnetic critical opalescence

Staatsexamens-Arbeit N. Thake 1999

Abbildung 5-6 Versuchsaufbau zur Messung der kritischen Streuung



$$\chi^+(T) \sim (T - T_C)^{-\gamma}$$
$$\chi^-(T) = \frac{1}{2} \chi^+(T)$$

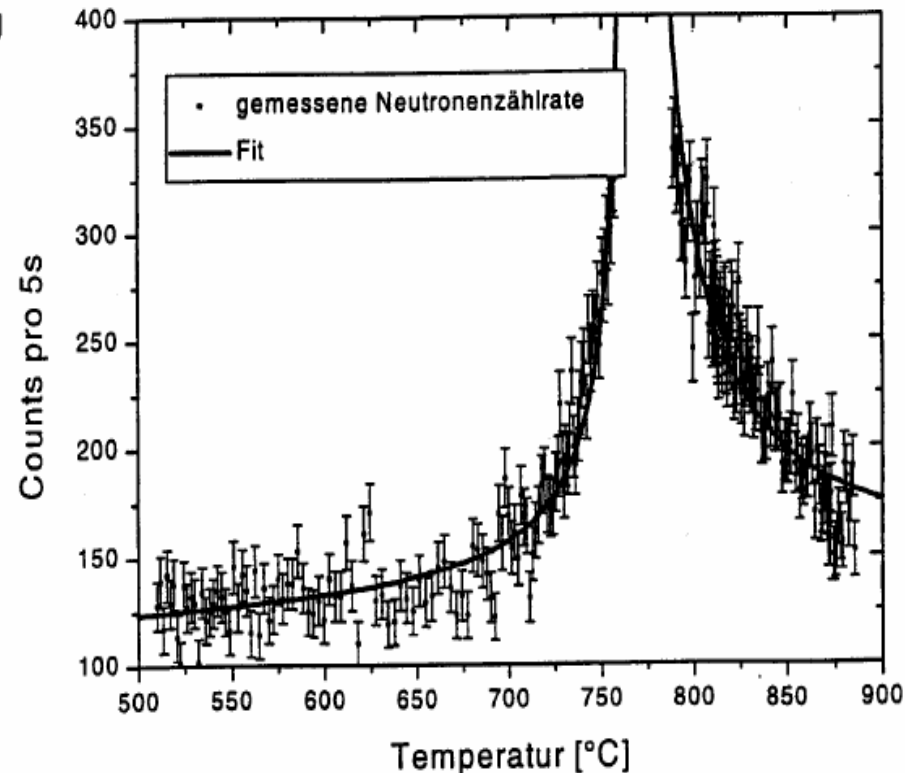


Abbildung 5-8 Messung der kritischen Streuung mit zugehörigem Fit

Correlation function near the critical point

For many systems the spatial correlation function decays with distance r like:

$$G(r) \sim \exp(-r/\xi)/r^n$$

Near the critical point ξ diverges like

$$\xi \sim |T - T_C|^{-\nu},$$

and the correlation function becomes

$$G(r) \sim 1/r^{d+2-\eta},$$

with dimension d , and with two further critical exponents ν and η .

Again, the critical exponents are not independent from each other.

In total, we will find, we need only two independent quantities.

At the moment, we note that empirically the following relations hold:

$$\alpha + 2\beta + \gamma = 2$$

$$\alpha + \beta(1 + \delta) = 2$$

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

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

so there are only 2 independent critical exponents.

11. Ising model

2 kinds of particles on a lattice, with next-neighbour (NN) interaction

Examples:

magnet:

↓↓↑↓↑↑↑↓↑↓

alloy:

●○○●○○●●

lattice gas:

○ · ○ · · ○ · ○ ○ ·

(=adatoms on surface)

Ferromagnet:

↓ ↓ ↑ ↓ ↓ ↑ ↑ ↑ ↓ ↑ ↓

$i:$ 1 2 3 ...

N spins s_i , (abbr. for s_{zi})

$s_i:$ - + - - + + + - + -

2^N possible configurations

Interaction energy for equal neighbours $E = -J$

Interaction energy for unequal neighbours $E = +J$, ($J = \text{const.}$)

$E/J:$ + - - + - + + - - -

" "

$s_i s_{i+1}:$ + - - + - + + - - -

and

$E = -J(+1-1-1+1-1+1+1-1-1-1)$ for this configuration

= Ising-Model with Hamiltonian

$$H = -J \sum_{i=1}^N s_i s_{i+1}$$

Example brass

From this we expect that an alloy should behave exactly like a ferromagnet,
what, indeed, it does.

Brass = copper-zinc alloy (55-90% Cu) $T < T_C = 733\text{K}$:

Order-disorder phase transition: ordered **below** T_C : ● ○ ● ○ ● ○ ● ○

unordered **above** T_C : ● ○ ○ ● ○ ● ● ○

(cf. melting point: $T_{Sm} \approx 1200\text{K}$)

Order parameter = difference in atomic sublattice concentration
measured via intensity I of a neutron Bragg-peak:

with reduced temperature $t = (T_C - T)/T_C$

order-parameter is

$$I = I_0 t^\beta$$

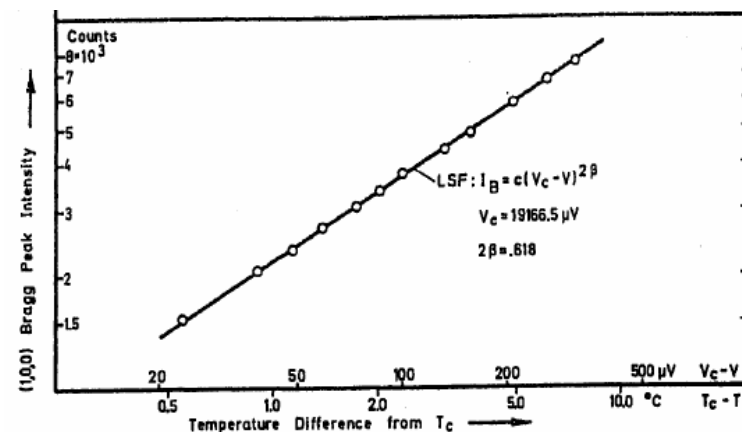
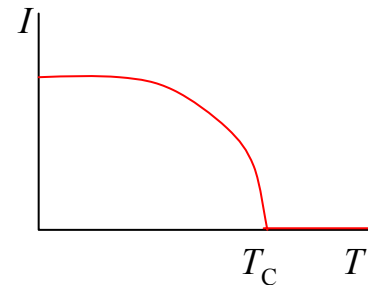
or

$$\log(I/I_0) = \beta \log t$$

with critical exponent β :

Experiment: $\beta = 0.31$ like 3-dim ferromagnet

(cf. 'mean field': $\beta = 1/2$)



J. Als-Nielsen (1976):

Phase Transitions Graduate Days
Oct. 2006

FIG. 4. Double log plot of the Bragg peak intensity versus the temperature difference $T_C - T$ or the thermocouple

Critical scattering from brass

From neutron small-angle scattering:
mean square fluctuation

$\langle n^2 \rangle - \langle n \rangle^2 \sim \chi =$ susceptibility:

$$\chi^+(T) \sim (T - T_C)^{-\gamma}$$

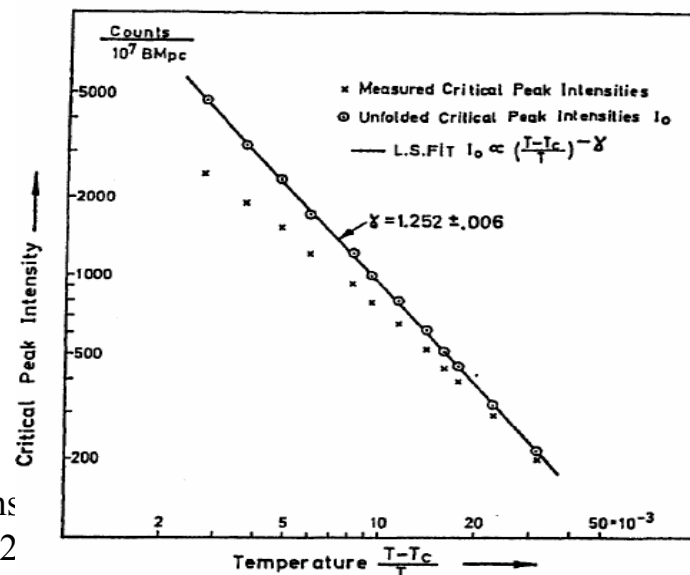
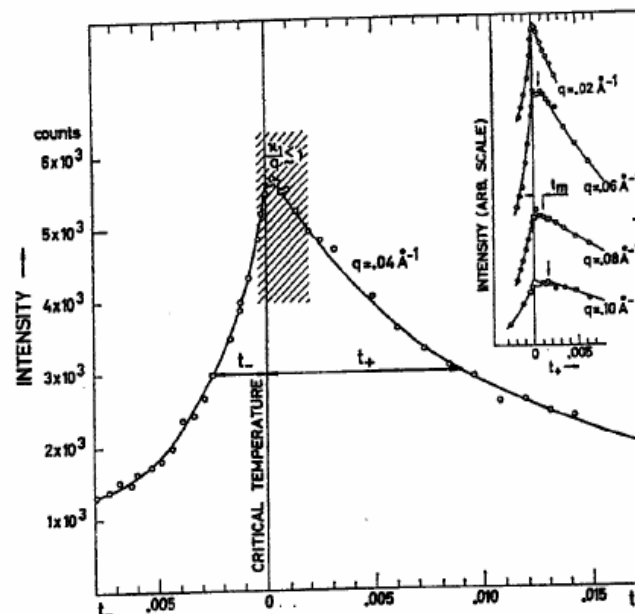
$$\chi^-(T) = \frac{1}{2} \chi^+(T)$$

or $\log \chi^\pm \sim -\gamma \log t$
 with critical exponent γ :

Experiment: $\gamma = 1.252(6)$
 like ferromagnet

(cf. 'mean field': $\gamma = 1$)

J. Als-Nielsen (1976):



a) Ising at $H=0$

1-dimensional Ising, NN-interaction:

Partition function under cyclic boundary conditions:

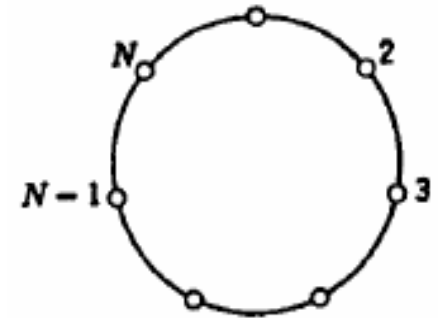
$$Z = \sum_{2^N \text{ config.}} \exp(-\hat{H}/kT)$$

$$Z = \sum_{s_1, s_2, \dots, s_N = \pm 1} \exp[(s_1 s_2 + s_2 s_3 + \dots + s_N s_1) J/kT]$$

$$Z = \sum_{\dots} \exp(s_1 s_2 J/kT) \times \exp(s_2 s_3 J/kT) \times \dots \times \exp(s_N s_1 J/kT),$$

with $s_i s_{i+1} = \pm 1$

$$Z = \sum \text{product of } \text{transfer matrix elements } V_{i i+1} = \exp(s_i s_{i+1} J/kT)$$



$n \times n$ transfer matrices

Transfer matrices

(V_{ij}) in general are $n \times n$ matrices if on each of N lattice sites n different configs:

Partition function

$$Z = \sum_{i,j,\dots,m=1,n} V_{ij} V_{jk} \cdots V_{mi}$$

(N indices \uparrow in n \uparrow configs.) (\uparrow product von N matrix elements)

Example: matrix element $V_{ij} = \exp(-\Phi_{ij}/kT)$, Φ_{ij} = potential, or $= s_i s_{i+1} J$ from prec. page

$$Z = \sum_{i=1,n} (V^N)_{ii} = \text{trace } V^N = \sum_{i=1,n} \lambda_i^N, \text{ with eigenvalues } \lambda_i \text{ of matrix } V.$$

Example $N=2$: element on the diagonal of V^N is $(V^2)_{ii} = \sum_{j=1,n} V_{ij} V_{ji}$,

from definition of matrix product

For particle number $N \gg 1$, and eigenvalue $\lambda_i \leq 1$:

only the largest eigenvalue λ_0^N of the transfer-matrix contributes as λ_0^N , i.e.

free energy $F = -kT \ln Z \approx -kT \ln \lambda_0^N = -vRT \ln \lambda_0$, with $Nk=vRT$.

Ising at $H=0$, spin $\frac{1}{2}$

1-dim, NN, $s = \frac{1}{2}$:

Transfer matrix

$$V = \begin{pmatrix} e^{J/kT} & e^{-J/kT} \\ e^{-J/kT} & e^{J/kT} \end{pmatrix}$$

With $x = J/kT$ transfer matrix V

has eigenvalues $\lambda_+ = e^x + e^{-x} = 2 \cosh x$

$$\lambda_- = e^x - e^{-x} = 2 \sinh x < \lambda_+$$

and eigenvectors $(-1, 1), (1, 1)$.

Partition function $Z \approx \lambda_+^N = (2 \cosh x)^N$:

free energy $F = -NkT \ln(2 \cosh x)$, mit $Nk = \nu R$

at low temperature $T = 0$, i.e. $x \rightarrow \infty$:

$$F \approx -NkT \ln e^x = -NkT x$$

$$F \approx -NJ$$

i.e. saturated ferromagnet:

↑↑↑↑↑↑↑↑

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$$m = \begin{pmatrix} e^x & e^{-x} \\ e^{-x} & e^x \end{pmatrix};$$

Eigenvalues[m] ;

Simplify[%]

$\{-e^{-x} + e^x, e^{-x} + e^x\}$

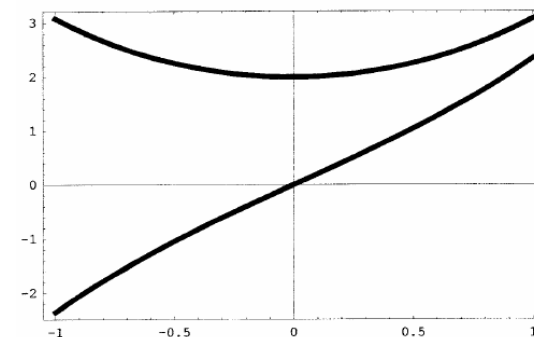
ExpToTrig[%]

$\{2 \sinh[x], 2 \cosh[x]\}$

Eigenvectors[m]

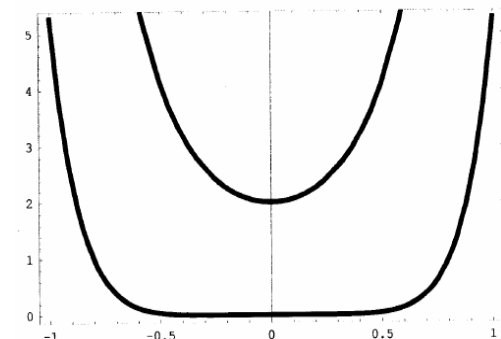
$\{\{-1, 1\}, \{1, 1\}\}$

Plot[{2 Sinh[x], 2 Cosh[x]}, {x, -1, 1}]



N = 6;

Plot[{2 Cosh[x]^N, 2 Sinh[x]^N}, {x, -1, 1}]



b) Ising at $H \neq 0$

1-dim, NN, $s = 1/2$:

Transfer matrix

$$V = \begin{matrix} \begin{matrix} s_{i+1} = 1 & -1 & s_i = \end{matrix} \\ \begin{pmatrix} e^{(J+H)/kT} & e^{-J/kT} \\ e^{-J/kT} & e^{(J-H)/kT} \end{pmatrix} \end{matrix} \begin{matrix} 1 \\ -1 \end{matrix}$$

with $x = J/kT$, $y = H/kT$ transfer matrix V

has eigenvalues $\lambda_{\pm} = e^x \cosh y \pm (e^{2x} \sinh^2 y + e^{-2x})^{1/2}$,

with maximum eigenvalue $\lambda_0 = \lambda_+$,

i.e. the free energy is $F \approx -NkT \ln \lambda_+$

Magnetization:

$$M = N \langle s \rangle = -\frac{\partial F}{\partial H} = \dots = N \frac{e^x \sinh y}{\sqrt{e^{2x} \sinh^2 y + e^{-2x}}}$$

Critical point in the Ising model

1-dim, NN, $s = 1/2$:

arbitrary temperature $T > 0$, magnetic field $H = 0$, i.e. $y = 0$:

Magnetization $\langle s \rangle = 0$

i.e. no spontaneous magnetization: **PM**

Temperature $T = 0$: spontaneous magnetization

$$\langle s \rangle \rightarrow e^x e^y / (e^{2x} e^{2y})^{1/2} \rightarrow \pm 1$$

for magnetic field $H \rightarrow 0^\pm$

$$\lim_{H \rightarrow 0^\pm} \lim_{T \rightarrow 0} \langle s \rangle = \pm 1$$

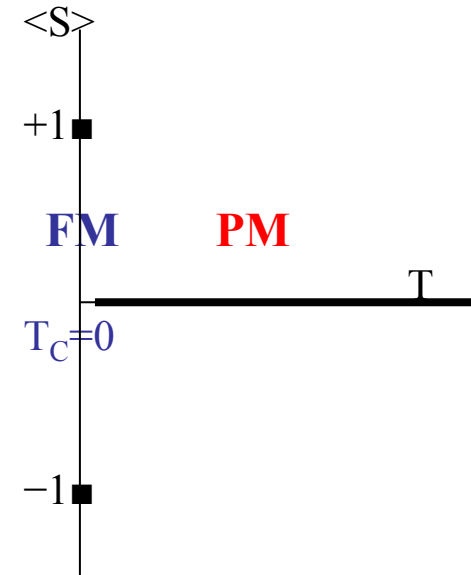
i.e. in the 1-dimensional Ising-Model there is
no phase transition at finite temperature $T > 0$,

the only phase transition **PM** \rightarrow **FM** being at $T_c = 0K$

Very general: There can be no long-range order in one dimension.

↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑ ↑

Destruction of long-range order with energy effort $\rightarrow 0$



Critical fluctuations in the Ising model

Spin-Spin correlation funktion in an isotropic and translationally invariant system was

$$G_R = \langle s_0 s_R \rangle - \langle s_0 \rangle \langle s_R \rangle.$$

At large distance R correlation decays as $G_R \sim \exp(-r/\xi)$.

i.e. correlation length ξ is given by

$$\xi^{-1} = \lim_{R \rightarrow \infty} [(-1/R) \ln G_R],$$

$$\xi^{-1} = \lim_{R \rightarrow \infty} [(-1/R) \ln |\langle s_0 s_R \rangle - \langle s_0 \rangle \langle s_R \rangle|],$$

$$\text{with } \langle s_0 s_R \rangle = Z_N^{-1} \sum_{\{s\}} s_0 s_R \exp(-\hat{H}_N/kT) \text{ etc.}$$

Using the transfer matrices one can show,

that for large N and for $R \rightarrow \infty$:

$$\xi^{-1} = -\ln (\lambda_1/\lambda_0),$$

with the largest and second-largest eigenvalues λ_0 und λ_1 .

Correlation function and length for $s=1/2$

for $s = 1/2$ the correlation length becomes:

$$\xi^{-1} = -\ln(\lambda_+/\lambda_-),$$

with the eigenvalues

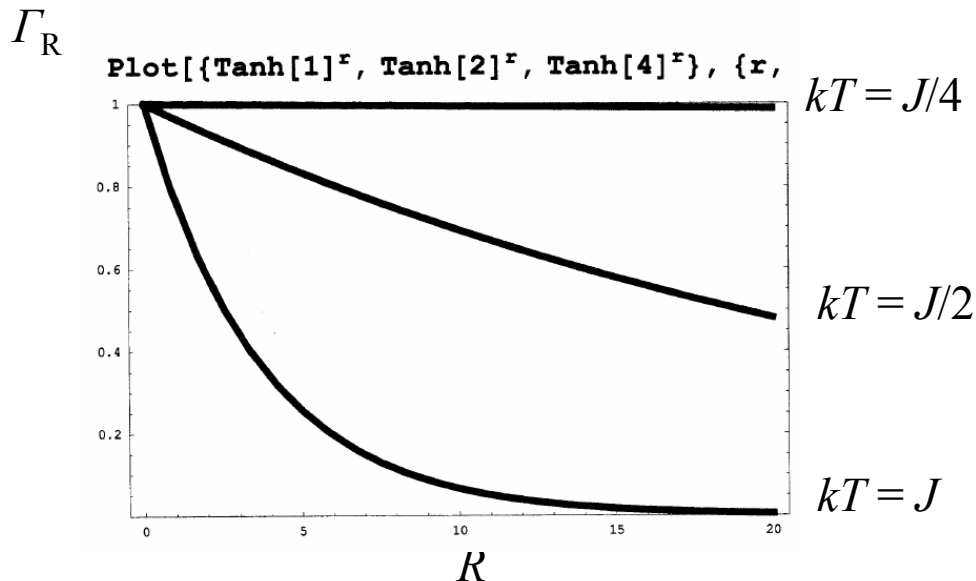
$$\lambda_{\pm} = e^x \cosh y \pm (e^{2x} \sinh^2 y + e^{-2x})^{1/2}$$

and

$$x=J/kT, y=H/kT$$

The correlation function in the limiting case $H = 0$ becomes:

$$\Gamma_R = \tanh^R(J/kT)$$



Ising models, state of the art

Dimension $d = 1$, spin $I = \frac{1}{2}$, field $H \neq 0$:	solved Ising 1925
Dimension $d = 2$, spin $I = \frac{1}{2}$, field $H = 0$:	solved Onsager 1944
Dimension $d = 2$, spin $I > \frac{1}{2}$, or field $H \neq 0$, or over-neighbor neighbours:	unsolved
Dimension $d = 3$:	unsolved
Dimension $d = 4$	\equiv mean field

12. Scale invariance and renormalization

Mean field: Averaging over all fluctuations is not permitted because fluctuation amplitudes diverge at the critical point.

Way out: successive averaging, separately for each scale, starting with a small length scale $L \ll$ coherence length ξ (when working in real space).

Example for $d = 2$ dimensional ('block-spin') iteration process:

Divide systems in blocks of volume $L^d = 3^2 = 9$ cells.

1. Take a majority vote in each block.
2. Combine the cells in a block and assign the majority vote to the cell.
3. Shrink new cells to the size of the original cells and renumber them. Number of configurations shrinks from $2^9 = 512$ to $2^1 = 2$.
4. 'Renormalize' the interaction \hat{H} between the averaged elements such that the new partition function stays the same:

$$Z_{N'} = \sum_{2^{N'} \text{ config.}} e^{-\beta \hat{H}'} = \sum_{2^N \text{ config.}} e^{-\beta \hat{H}} = Z_N,$$

so that the physics remains the same (scale invariance). Go to 1.

+	-	+	+	-	-	+	+	-
-	-	+	-	+	+	-	+	-
+	+	-	-	+	+	-	-	
-	+	-	+	-	-	-	+	-
+	-	-	+	+	+	+	-	+
+	+	-	-	-	+	+	-	+
+	-	+	-	+	-	-	+	-
-	+	-	+	+	-	+	+	-
+	-	+	+	-	-	+	-	-

+	+	-
-	+	+
+	-	-

+	+	-
-	+	+
+	-	-

Block-spin operation in 2-dim.

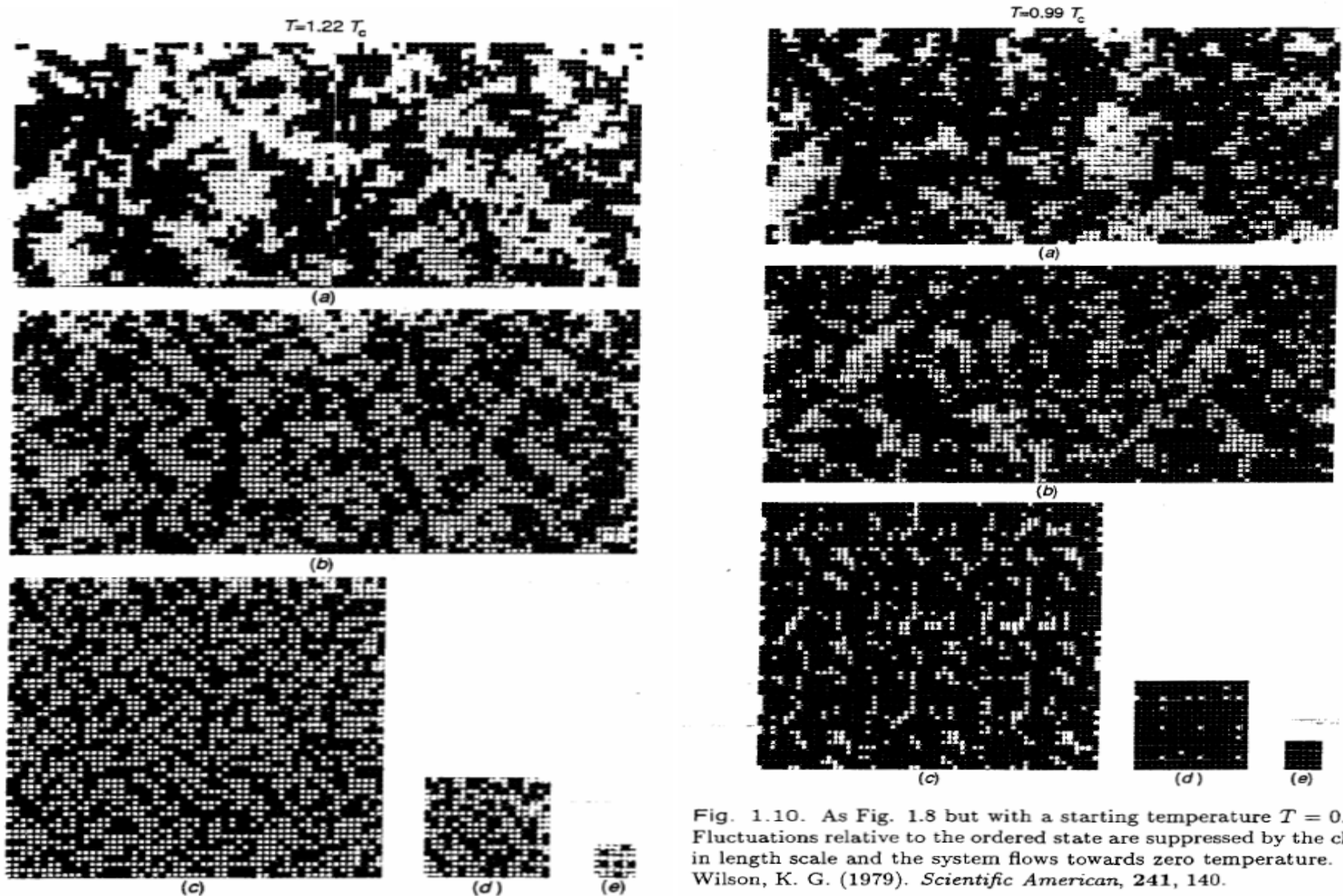


Fig. 1.10. As Fig. 1.8 but with a starting temperature $T = 0.99 T_c$. Fluctuations relative to the ordered state are suppressed by the change in length scale and the system flows towards zero temperature. After Wilson, K. G. (1979). *Scientific American*, 241, 140.

Block-spin operation in 2-dim.: $T=T_c$

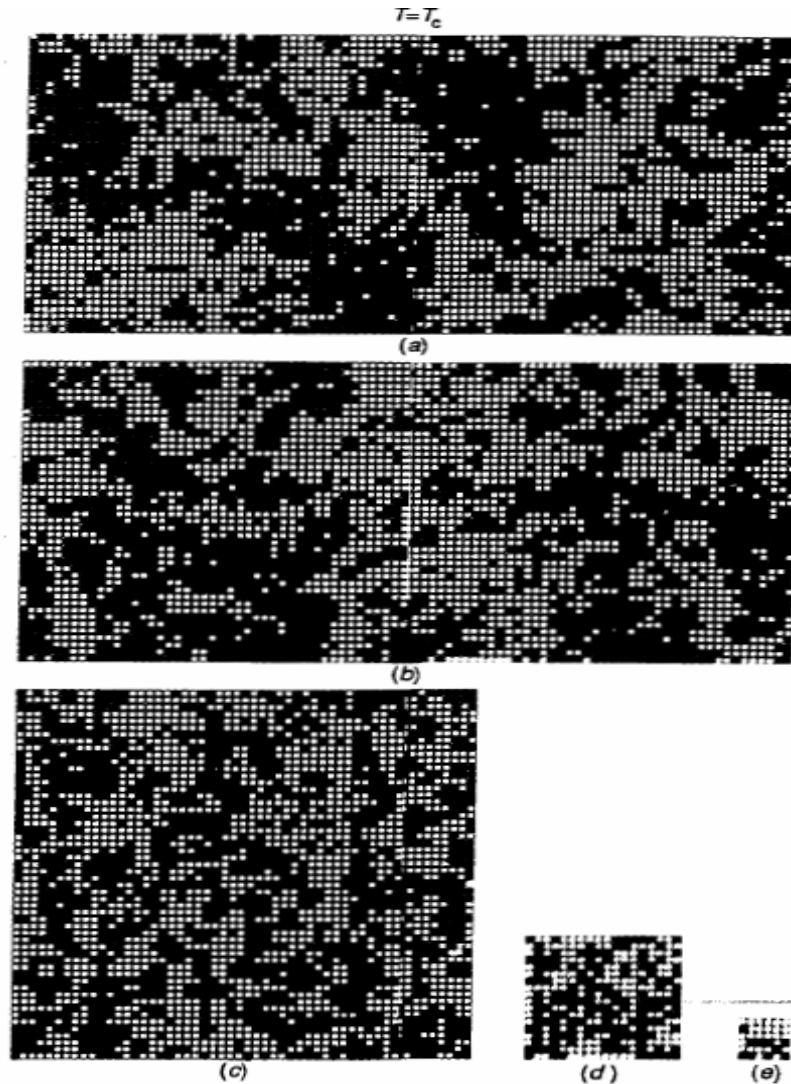


Fig. 1.9. As Fig. 1.8 but with a starting temperature $T = T_c$. Because the correlation length is initially infinite there is no change in the ordered state under iteration of the renormalization group and the system remains at the critical temperature. After Wilson, K. G. (1979). *Scientific American*, 241, 140.

Transformation of reduced temperature and field

At each iteration step:

coherence length shrinks from ξ to $\xi' = \xi / L$,

that is temperature T moves away from T_C ,

either to higher $T \rightarrow \infty$ or to lower $T \rightarrow 0$ temperatures:

Under an iteration the reduced temperature $t = |(T - T_C)/T_C|$ changes from t to $t' = g(L) t$, the function $g(L)$ is to be determined:

Upon two iterations, successive shrinking is by L_1 , then by L_2 , in total by $L_1 L_2$.

Reduced temperature changes to $t' = g(L_2) g(L_1) t = g(L_1 L_2) t$.

A function with the property $g(L_2) g(L_1) = g(L_1 L_2)$ necessarily has the form $g(L) = L^y$,

Check: $L_1^y L_2^y = (L_1 L_2)^y$.

Hence the reduced temperature t transforms as: $t' = L^y t$ with exponent $y > 0$.

Same argument for magnetic field: it increases when coherence length shrinks:

i.e. reduced field h transforms as: $h' = L^x h$ with exponent $x > 0$.

Critical exponent relations from scaling

During shrinking, densities increase by L^d ,
in particular free energy density f grows as:

$$f(t', h') = L^d f(t, h),$$

$$\text{or } f(t, h) = L^{-d} f(L^y t, L^x h).$$

From this property of the free energy
we can derive the relations
between the critical exponents:

1. Order parameter magnetization:

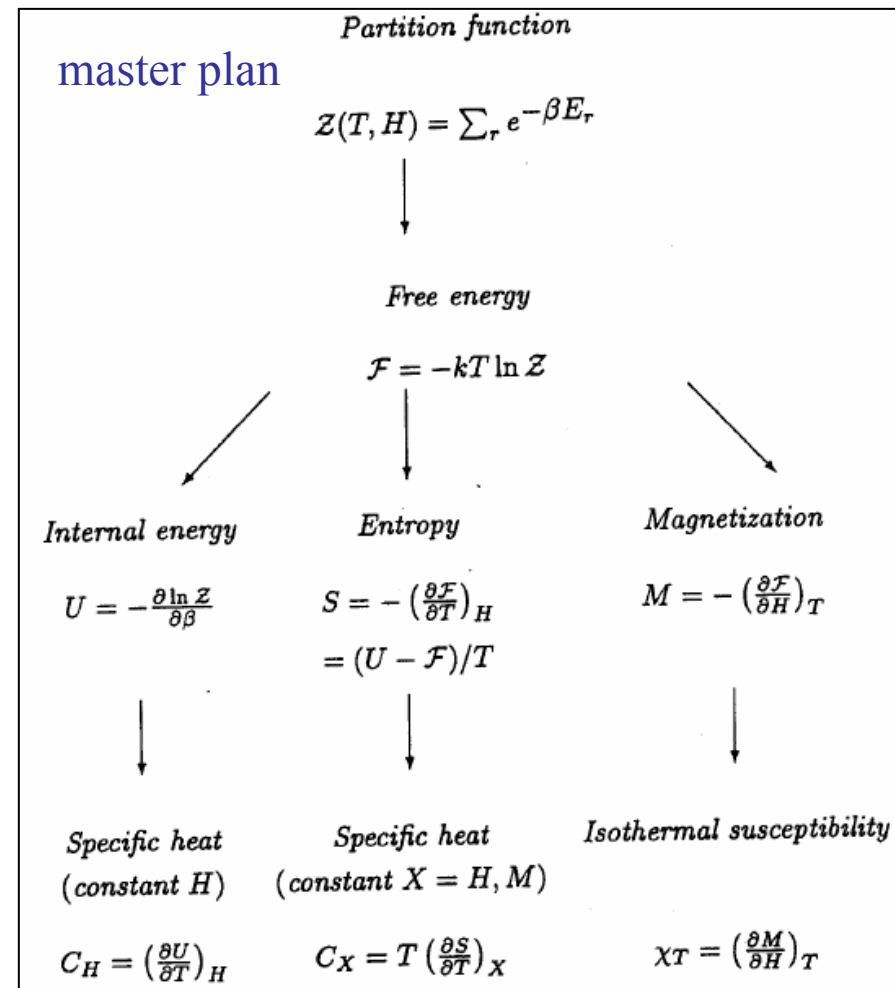
$$m = -\partial f(t, h) / \partial h|_{h \rightarrow 0}$$

$$= L^{-d} L^x \partial f(L^y t, L^x h) / \partial h|_{h \rightarrow 0};$$

this holds for any L , in particular for
 $|L^y t| = 1$, i.e. $L = t^{-1/y}$:

$$m = |t|^{(d-x)/y} \partial f(\pm 1, 0) / \partial h = \text{const.} |t|^\beta,$$

with critical exponent $\beta = (d - x)/y$.



Critical exponent relations from scaling

With similar arguments:

2. Susceptibility $\chi = -\partial^2 f(t, h)/\partial h^2|_{h \rightarrow 0} \sim |t|^{-\gamma}$,
with critical exponent $\gamma = (2x - d)/y$
3. Critical isotherm $m = -\partial f(t, h)/\partial h|_{t \rightarrow 0} \sim |h|^{1/\delta}$
with critical exponent $\delta = x/(d - x)$
4. Specific heat ($h=0$) $C_V = -\partial^2 f(t, 0)/\partial t^2 \sim |t|^{-\alpha}$
with critical exponent $\alpha = 2 - d/y$
5. Coherence length $\xi \sim |t|^{-\nu}$
with critical exponent $\nu = 1/y$
6. Correlation function $G \sim 1/r^{d-2+\eta}$
with critical exponent $\eta = 2 + d - 2x$

which can in principle be resolved to write all
critical exponents as functions of two variables x and y .

Renormalization

In each iteration step the Hamiltonian is renormalized:

$$\hat{H}' = R(\hat{H}), \hat{H}'' = R(\hat{H}'), \text{ etc.,}$$

and with each step in parameter space (t, h)

one moves further away from the critical temperature T_C (or $t = 0$).

Find in parameter space the point where \hat{H} is a fixed point under R:

$$\hat{H}^* = R(\hat{H}^*).$$

There, also temperature and field are fixed points under R:

$$t^* = L^y t^*, h^* = L^x h^* \text{ for all } L:$$

i.e.: $t^* = 0$ ($T = T_C$), and $h^* = 0$

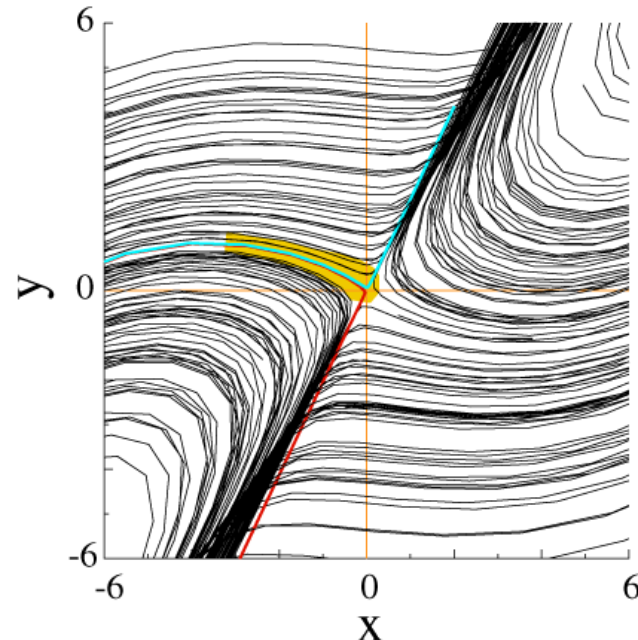
(or $t^* = \infty, h^* = \infty$ at $T = \infty$).

At T_C the correlation length ξ no longer changes under R:

$$\xi^* = \xi^*/L \text{ for all scales } L, \text{ so } \xi^* = \infty \text{ at } T_C$$

(or $\xi^* = 0$ for $T \rightarrow \infty$).

Investigate the iteration trajectories near this fixed points
and derive from them the critical exponents.



The universality classes of continuous phase transit.

The critical exponents depend on only two paramters x and y .

Can these take any value?

No, because they can be shown to depend only on two other geometrical entities:

1. the spatial dimensionality d of the system
2. the dimensionality n of the order parameter

Example: Magnetization M :

$n = 1$: Ising model $s_z = \pm 1$ in $d = 1, 2, 3$ dimensions

$n = 2$: xy-model with planar spin M_{xy} moving in x-y plane

$n = 3$: Heisenberg model with 3-vector \mathbf{M} .

As d and n are discrete numbers, there is a countable number of universality classes (d, n) , and within each class the critical behaviour in continuous phase transitions is identical.

Values of the critical exponents for (d, n)

with $\epsilon = 4 - d$:

$$\gamma = 1 + \frac{n+2}{2(n+8)} \epsilon + \dots, \quad (7.1)$$

$$\beta = \frac{1}{2} - \frac{3}{2(n+8)} \epsilon + \dots, \quad (7.2)$$

$$\alpha = \frac{4-n}{2(n+8)} \epsilon + \frac{(n+2)^2(n+28)}{4(n+8)^3} \epsilon^2 + \dots, \quad (7.3)$$

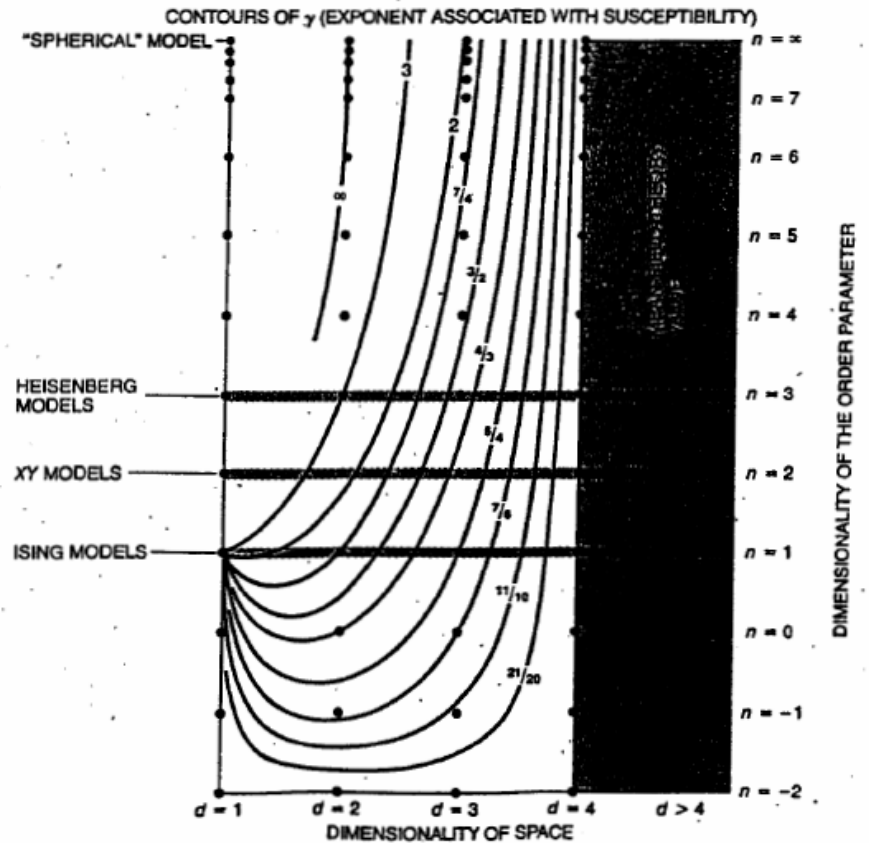
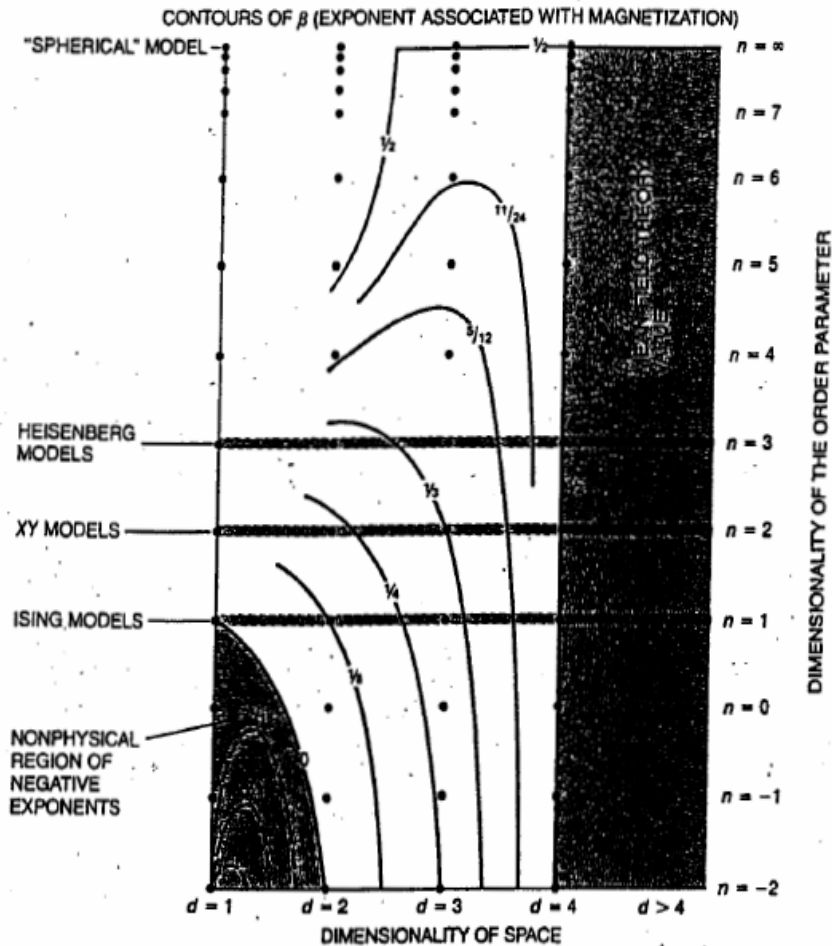
$$\eta = \frac{n+2}{2(n+8)^2} \epsilon^2 + \dots, \quad \delta = 3 + \epsilon + \dots, \quad (7.4)$$

The higher the dimension, the less the system is disturbed by fluctuations.

(example: Domino in various dimensions)

For $d = 4$, we are back at the mean field results.

Critical exponents β and γ



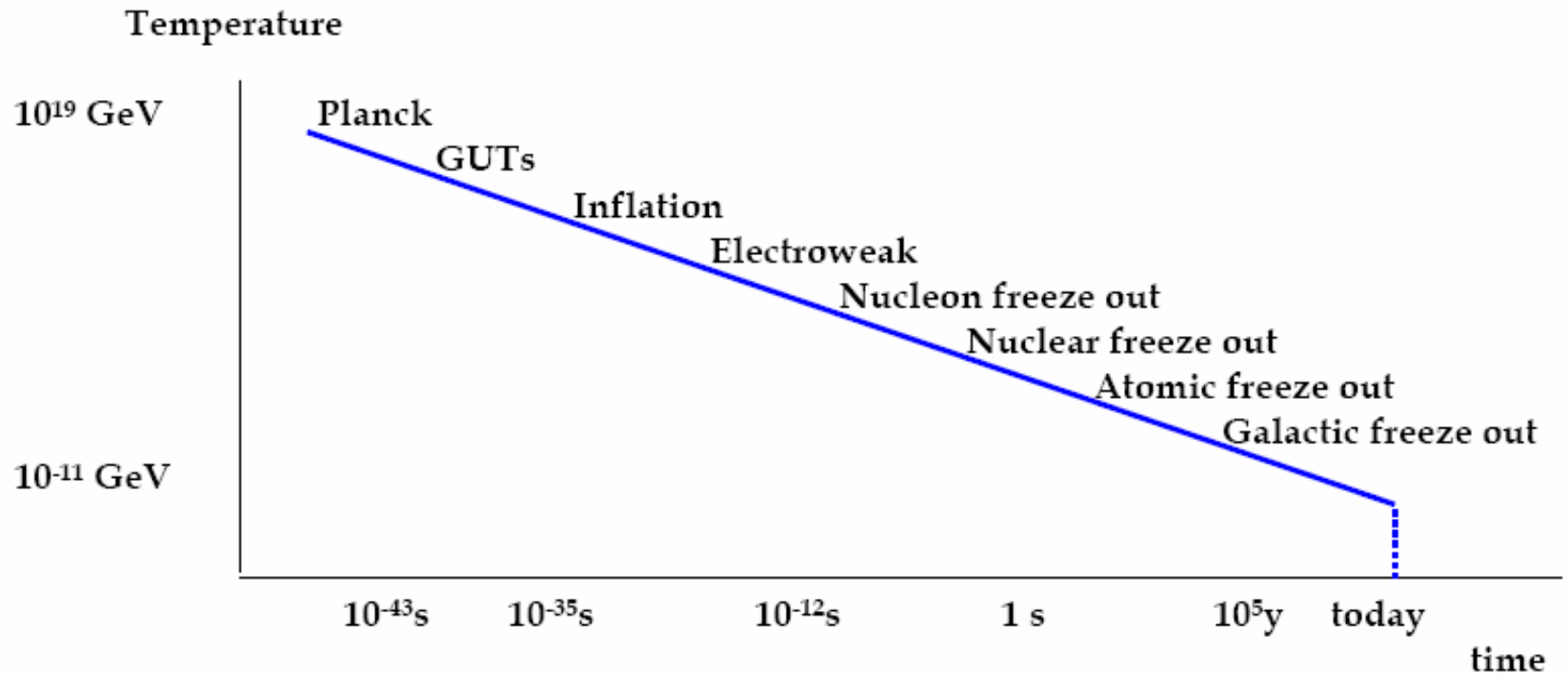
VARIATION OF CRITICAL EXPONENTS with the dimensionality of space (d) and of the order parameter (n) suggests that physical systems in different universality classes should have different critical properties. The exponents can be calculated as continuous functions of d and n , but only systems with an integral number of dimensions are physically possible. In a space with four or more dimensions all the critical exponents take on the values predicted by mean-field theories. The graphs were prepared by Michael E. Fisher of Cornell University.

Well known universality classes

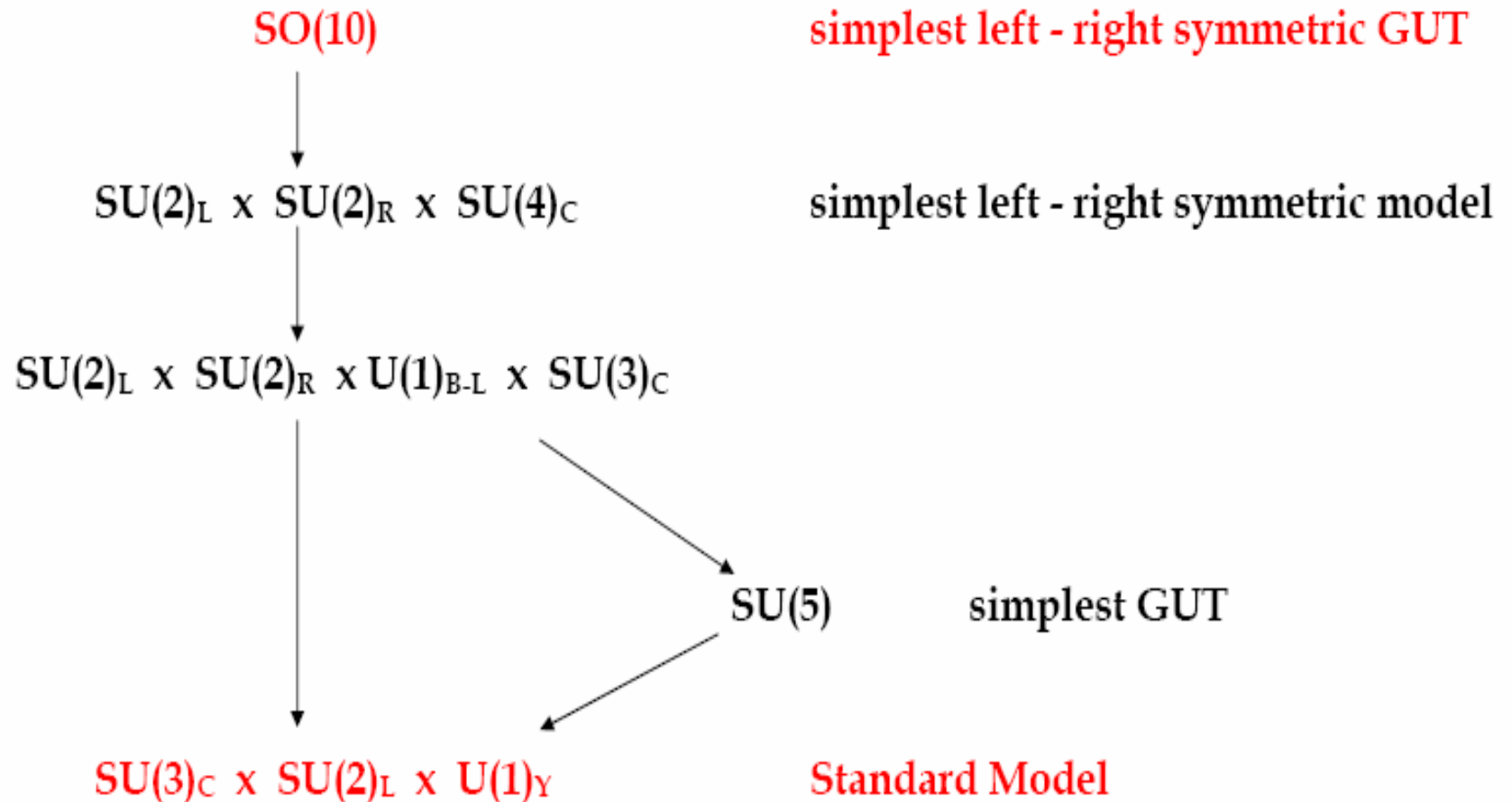
Table 3.1. Universality classes

Universality class	Symmetry of order parameter	α	β	γ	δ	ν	η	Physical examples
2-d Ising	2-component scalar	0 (log)	1/8	7/4	15	1	1/4	some adsorbed mono e.g. H on Fe
3-d Ising	2-component scalar	0.10	0.33	1.24	4.8	0.63	0.04	phase separation, flu order-disorder e.g. β
3-d X-Y	2-dimensional vector	0.01	0.34	1.30	4.8	0.66	0.04	superfluids, supercon
3-d Heisenberg	3-dimensional vector	-0.12	0.36	1.39	4.8	0.71	0.04	isotropic magnets
mean-field		0 (dis.)	1/2	1	3	1/2	0	
2-d Potts, $q=3$ $q=4$	q -component scalar	1/3 2/3	1/9 1/12	13/9 7/6	14 15	5/6 2/3	4/15 1/4	some adsorbed mono e.g. Kr on graphite

13. Phase transitions in the universe



A possible GUT symmetry breaking chain



Inflation

Lit. A. Linde: Particle physics and inflationary cosmology.

Inflation:

If Hubble constant is not a constant, $H = \dot{a}/a = \text{const.}$,
then there automatically is inflation: $a = a_0 e^{Ht}$.

But $H \neq \text{const.}$: $(\dot{a}/a)^2 + k/a^2 = (8\pi/3) G\rho$

Hot big bang model: solution $a(t) \sim t^{1/2}$ relativistic
 solution $a(t) \sim t^{3/2}$ today

Flat universe for $k = 0$, i.e. $\rho = \rho_C = 3H^2/8\pi G$
i.e. $\Omega = \rho/\rho_C = 1$

Flat universe

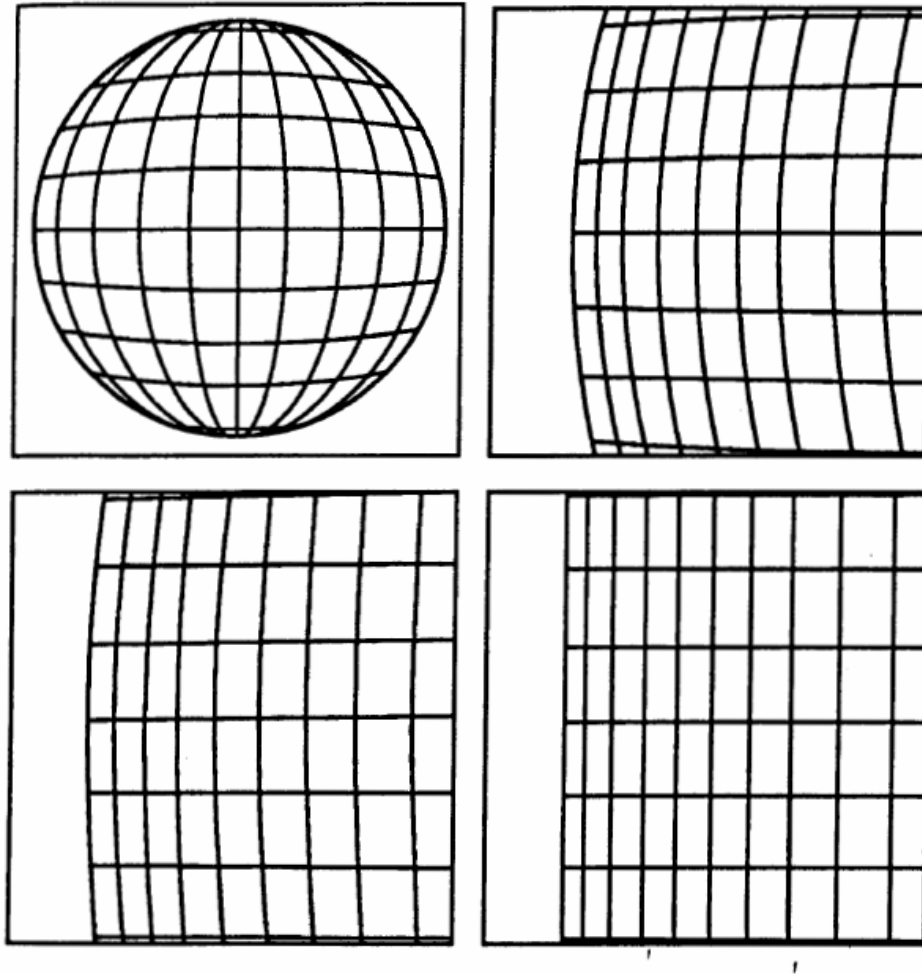


Figure 7. When an object increases enormously in size, its surface geometry becomes almost Euclidean. This effect is fundamental to the solution of the flatness, homogeneity, and isotropy problems in the observable part of the universe, by virtue of the exponentially rapid inflation of the latter.

Inflation mechanism

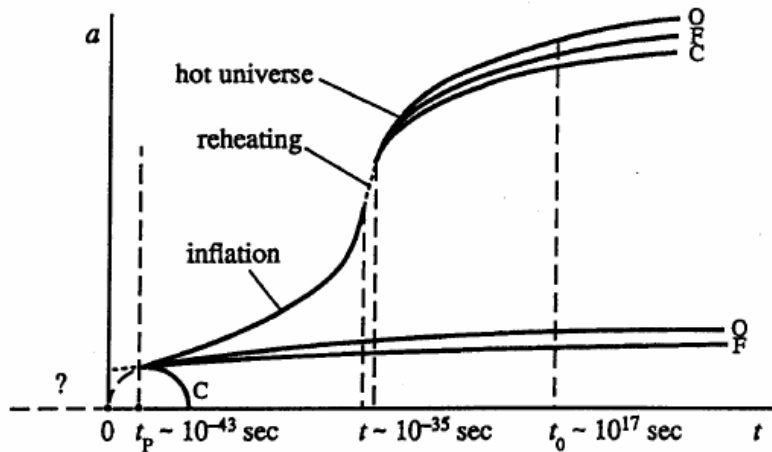


Figure 6. The lighter set of curves depicts the behavior of the size of the hot universe (or more precisely, its scale factor) for three Friedmann models: open (O), flat (F), and closed (C). The heavy curves show the evolution of an inflationary region of the universe. Because of quantum gravitational fluctuations, the classical description of the expansion of the universe cannot be valid prior to $t \sim t_p = M_P^{-1} \sim 10^{-43}$ sec after the Big Bang at $t = 0$ (or after the start of inflation in the given region). In the simplest models, inflation continues for approximately 10^{-35} sec. During that time, the inflationary region of the universe grows by a factor of from 10^{17} to $10^{10^{14}}$. Reheating takes place afterwards, and the subsequent evolution of the region is described by the hot universe theory.

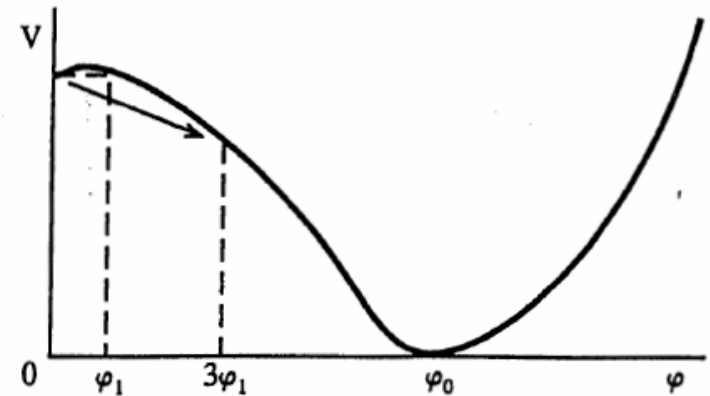
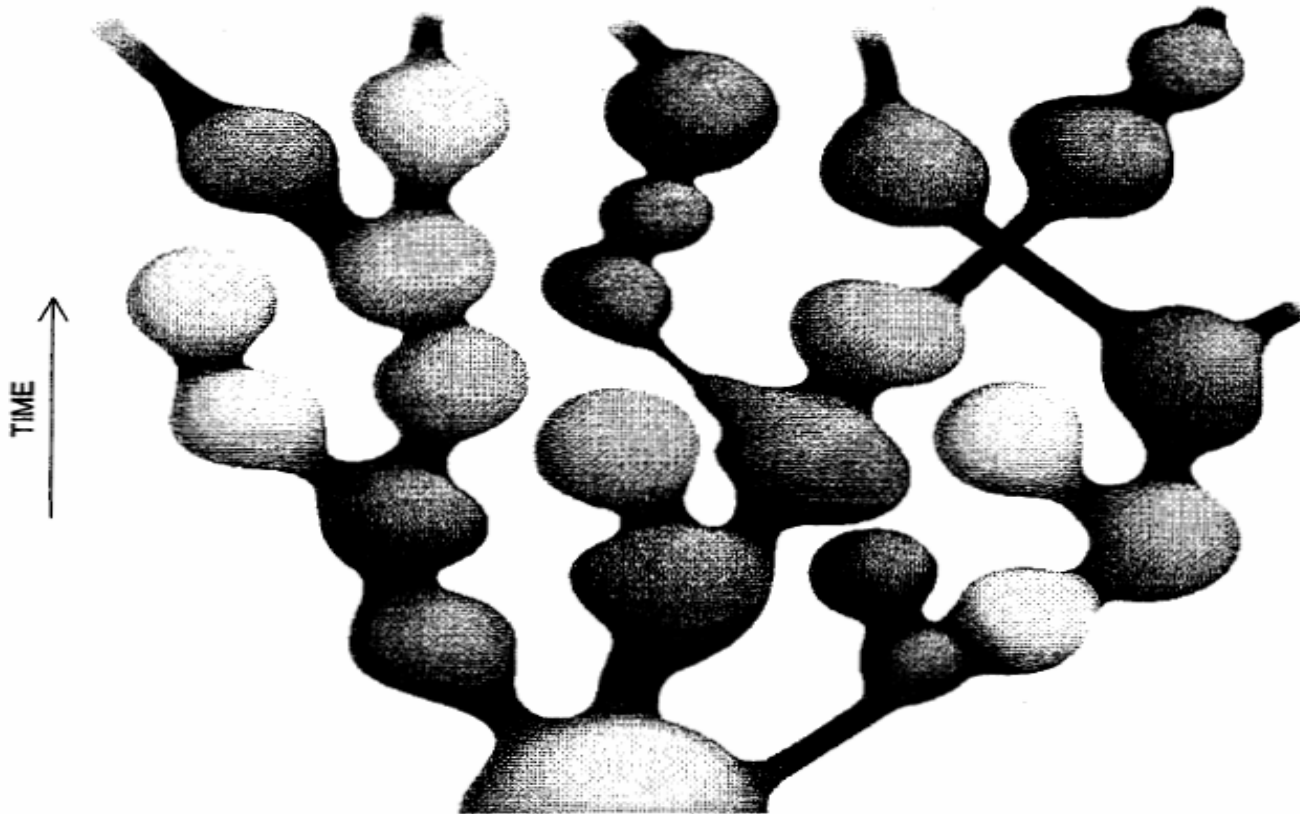


Fig. 34. Effective potential in the Coleman–Weinberg theory at finite temperature. Tunneling proceeds via formation of bubbles of the field $\phi \leq 3\phi_1$, where $V(\phi_1, T) = V(0, T)$.

Self reproducing cosmos



SELF-REPRODUCING COSMOS appears as an extended branching of inflationary bubbles. Changes in color represent "mutations" in the laws of physics from parent universes. The properties of space in each bubble do not depend on the time when the bubble formed. In this sense, the universe as a whole may be stationary, even though the interior of each bubble is described by the big bang theory.