G. Mean-field Theory: A systematic formalism

$$H_{exact} \rightarrow H_{(approx.)} \rightarrow Z_{approx} \rightarrow F \rightarrow \text{other quantities}$$

Ising Model: $$E(\{S_i\}) = -J \sum_{\langle ij \rangle} S_i S_j - B \sum_i S_i \quad (1)$$

used $E(\{S_i\})$ here

to emphasize that given a pattern of "+1" and "−1" of all sites, there follows an energy $E(\{S_i\})$ for the N-spin state, and this $E(\{S_i\})$ goes into $Z = \sum_{\text{all possible } \{S_i\}} e^{-E(\{S_i\})/kT}$

(more often, it is written as H, for Hamiltonian)

Mean-field approximation: "S_i is only slightly different from $\langle S_i \rangle$"

Write: $$S_i = S_i - \langle S_i \rangle + \langle S_i \rangle = \langle S_i \rangle + (S_i - \langle S_j \rangle)$$

$$E_{interaction}(\{S_i\}) = -J \sum_{\langle ij \rangle} S_i S_j = -J \sum_{\langle ij \rangle} (S_i - \langle S_i \rangle + \langle S_i \rangle)(S_j - \langle S_j \rangle + \langle S_j \rangle)$$

$$= -J \sum_{\langle ij \rangle} \Big[(S_i - \langle S_i \rangle)\langle S_j \rangle + (S_j - \langle S_j \rangle)\langle S_i \rangle + \langle S_i \rangle \langle S_j \rangle + \underbrace{(S_i - \langle S_i \rangle)(S_j - \langle S_j \rangle)}_{\text{ignore this term (thus avoided } S_i S_j \text{ term)}} \Big]$$

$$E_{int}^{(MF)}(\{S_i\}) \approx -J \sum_{\langle ij \rangle} \Big[(S_i - \langle S_i \rangle)\langle S_j \rangle + (S_j - \langle S_j \rangle)\langle S_i \rangle + \langle S_i \rangle \langle S_j \rangle \Big] \quad (16)$$

$\langle S_i \rangle$, $\langle S_j \rangle$ ↑ numbers to be determined self-consistently

$B = 0$ (no applied field) <u>OR</u> uniform B ($B_{applied}$ is the same[+] everywhere), spin at i (or spin at j or any location) is nothing special, so

expect $\langle S_i \rangle = \langle S_j \rangle = \langle S \rangle_{\text{any location}} \equiv m$ ← to be determined

---

[+] An interesting variation on the Ising Model is the Random field Ising Model with $B_{applied,i}$ depending on location.

$$E_{int}^{(MF)}(\{S_i\}) = -J \sum_{\langle ij \rangle} \left[(S_i - m)m + (S_j - m)m + m^2 \right]$$

$$= -2Jm \underbrace{\sum_{\langle ij \rangle} S_i}_{\text{like a field interacting with independent spins}} + J \sum_{\langle ij \rangle} m^2 \qquad (17)$$

$\sum_{\langle ij \rangle} S_i = \frac{z}{2} \sum_i S_i$

over distinct n.n. pairs

over all spins (moments)

there are z neighbors

$\Rightarrow$ z pairs (in sum) involve i

$$\sum_{\langle ij \rangle} S_i = \frac{z}{2} \sum_{i=1}^{N} S_i \qquad (18)$$

over sites (over individual spins)

correct for double-counting (RHS will go over i and go over j)

Similarly, $J \sum_{\langle ij \rangle} m^2 = Jm^2 \sum_{\langle ij \rangle} 1 = Jm^2 \frac{z}{2} N$

$$\therefore \quad E_{int}^{(MF)}(\{S_i\}) = -zJm\sum_{i=1}^{N} S_i + N\frac{Jz}{2}m^2$$

General case with $B_{applied} \neq 0$, add back $-B\sum_{i=1}^{N} S_i$,

$$\boxed{E_{Ising}^{(MF)} = -(Jzm + B)\sum_{i=1}^{N} S_i + N\frac{Jz}{2}m^2} \qquad (19)$$

internal mean-field (but m is unknown) external field just a constant (but m is the unknown)

This is the Mean-field Hamiltonian (H_{MF})

Next, we follow stat. mech. approach, i.e. find $Z_{MF} \to F_{MF}$, etc.

(but it is just like a paramagnetism problem)

$$Z_{MF} = \sum_{\text{all strings } \{S_i\}} e^{-E^{(MF)}(\{S_i\})/kT} = e^{\frac{-NJzm^2}{2kT}} \sum_{\text{all strings } \{S_i\}} e^{(Jzm+B)\left(\sum_{i=1}^{N} S_i\right)/kT}$$

$$= e^{\frac{-NJzm^2}{kT}} \sum_{S_1=+1,-1} \sum_{S_2=+1,-1} \cdots \sum_{S_N=+1,-1} e^{\frac{(Jzm+B)}{kT}(S_1+S_2+\cdots+S_N)}$$

equivalent to sum over all strings $\{S_i\}$ (same as two-level systems)

$$= e^{-\frac{NJzm^2}{kT}} \left(\sum_{S_i=+1,-1} e^{\frac{(Jzm+B)}{kT} S_i} \right)^N$$

$$= e^{-\frac{NJzm^2}{kT}} \left(2\cosh\left(\frac{Jzm+B}{kT}\right)\right)^N$$

$$= \left[2\, e^{-\frac{Jzm^2}{kT}} \cosh\left(\frac{Jzm+B}{kT}\right)\right]^N = z^N \qquad (20)$$

(same steps as in two-level/paramagnetism problems)

$$F_{MF} = -kT \ln Z_{MF} = N\cdot(-kT\ln z) \equiv N\cdot f_{MF}$$ ← Helmholtz free energy per spin (within MF theory)

$$\boxed{f_{MF} = -kT\ln\left[2\cosh\left(\frac{Jzm+B}{kT}\right)\right] + \frac{Jzm^2}{2}} \qquad (21)$$

Key Result

Note that $f_{MF}(T,B)$, we also expect m to depend on B.

$$m = -\left(\frac{\partial f}{\partial B}\right)_T = -Jzm\left(\frac{\partial m}{\partial B}\right)_T + kT\,\frac{2\sinh\left[\frac{Jzm+B}{kT}\right]}{2\cosh\left[\frac{Jzm+B}{kT}\right]}\cdot\left(\frac{Jz\left(\frac{\partial m}{\partial B}\right)_T + 1}{kT}\right)$$

susceptibility → $\sim\chi$

$$= Jz\cdot\underbrace{\left(\frac{\partial m}{\partial B}\right)_T}_{\sim\chi}\left[-m + \tanh\left[\frac{Jzm+B}{kT}\right]\right] + \tanh\left[\frac{Jzm+B}{kT}\right]$$

$$\Rightarrow \underbrace{\left[1 + Jz\left(\frac{\partial m}{\partial B}\right)_T\right]}_{\text{positive }(\neq 0)}\left[\tanh\left[\frac{Jzm+B}{kT}\right] - m\right] = 0$$

to solve for m

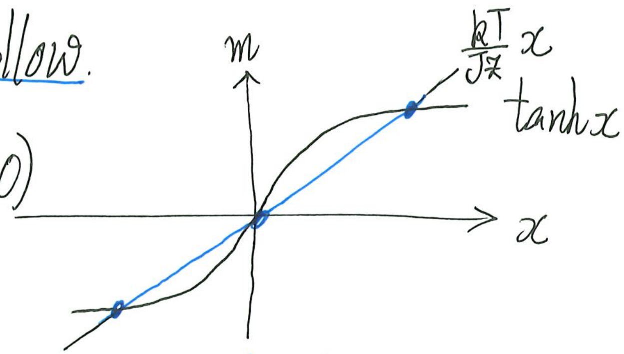
$\therefore$ m is determined by $$\boxed{m = \tanh\left[\frac{Jzm + B}{kT}\right]} \quad (22)$$

this is the Mean-field equation Eq. (4) in Sec. F

then all results in Sec. F follow.

- But we gained something. Recall $T < T_c$ $(B=0)$

$$m = \tanh\left(\frac{Jz}{kT} m\right)$$



3 roots for m

> Which root(s) is (are) the physical root(s)?
>
> Plug root (m) into f , identify the one(s) that minimize f.

- Can get $\langle E \rangle_{\text{per spin}}$ from $-\frac{\partial}{\partial \beta} \ln z$, then study heat capacity as $T \to T_c^+$ and $T \to T_c^-$.
- How about susceptibility χ for $T \to T_c^+$?

Summary

- The mean field equation $m = \tanh\left(\frac{Jzm}{kT} + \frac{B}{kT}\right)$ can be obtained in many ways, e.g. physical argument and statistical mechanics formula.
- MFT gives critical phenomena
- However, critical exponents β, δ, γ predicted by MFT are often not accurate.

	2D	3D	4D	MFT
β	$1/8$	0.326	$1/2$	$1/2$
δ	15	4.790	3	3
γ	$7/4$	1.237	1	1

- MF results are off in 2D, 3D
- MF results agree with 4D results!
- Higher dimensions, what are ignored in MF turned out to be something that can be ignored!
- 4D is the "upper critical dimension" of Ising Model

References

- K. Huang, "Statistical Mechanics" (this is a chapter on Ising Model)
- K. Christensen and N.R. Moloney, "Complexity and Criticality"
  (Ch. 2 is about the Ising Model, there are only three chapters)

$\underbrace{\text{Percolation, Ising Model, Selforganised Criticality}}_{\text{three very interesting topics in statistical physics}}$

H. Looking at f as a function of m: A twist of important consequences

$$f = \frac{Jz m^2}{2} - kT \ln\left[2\cosh\left(\frac{Jz m}{kT} + \frac{B}{kT}\right)\right] \quad (21)$$

Motivation:

When MF equation gives multiple roots, m should be the one(s) that minimizes f

Hints at regarding f as $f(m, T)$?

m ← order parameter

How about setting $\left(\frac{\partial f}{\partial m}\right)_{T,B} = 0$?

$$\frac{\partial f}{\partial m} = Jzm - kT \frac{2\sinh\left(\frac{Jzm+B}{kT}\right)}{2\cosh\left(\frac{Jzm+B}{kT}\right)} \cdot \frac{Jz}{kT}$$

$$= Jz\left[m - \tanh\left(\frac{Jzm+B}{kT}\right)\right]$$

$\frac{\partial f}{\partial m} = 0$ gives $\underbrace{m = \tanh\left[\frac{Jzm+B}{kT}\right]}_{\text{the MF equation!}}$

∴ Take f and view it as $f(m,T)$, and inspect its minimum is meaningful!

To get prepared, we note that $f(T\to\infty) = -kT\ln 2 \equiv \bar{f}$

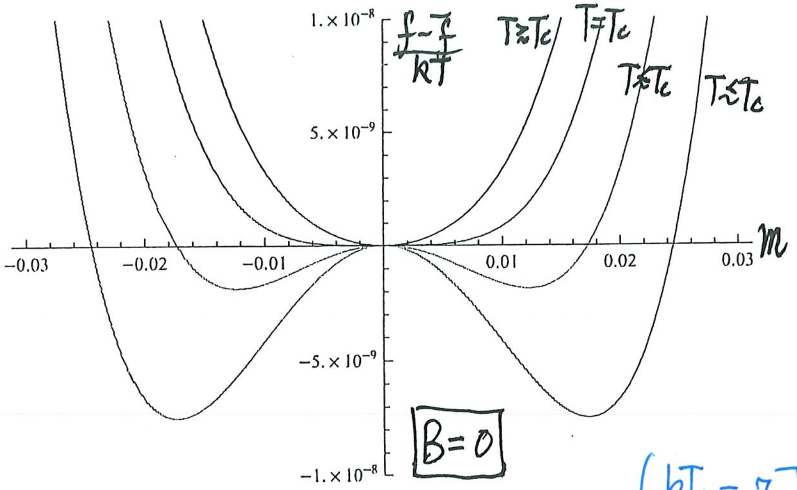
$\uparrow$ $(+1 \text{ or } -1)$ (2 choices)

Consider $f - \bar{f} = \dfrac{Jzm^2}{2} - kT\ln\left[2\cosh\left(\dfrac{Jzm}{kT} + \dfrac{B}{kT}\right)\right] \underbrace{+\, kT\ln 2}_{\text{just a constant}}$

[added in $\bar{f}$ into the "f" previously]

$B=0,\quad f - \bar{f} = \dfrac{Jzm^2}{2} - kT\ln\left[2\cosh\left(\dfrac{Jzm}{kT}\right)\right] + kT\ln 2$

Regard $(f-\bar{f})$ as a function of m



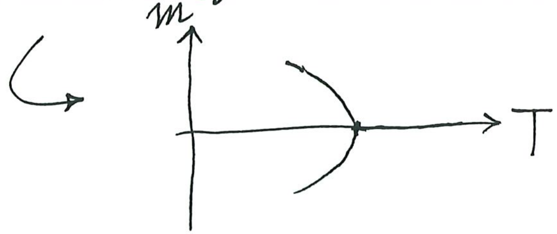
$(kT_c = zJ)$

$T > T_c$: $m=0$ is a minimum

$T = T_c$: $m=0$ is a minimum and curve becomes rather flat near $m=0$

$T \lesssim T_c$: $m=0$ is a **maximum** and two other values ($\pm$) are minima

Tracing the minima:



Key Features

$f(m)$ [or $f-\bar{f}$] changes qualitatively as T passes through T_c

$T > T_c$, $m=0$ gives minimum f [as well as $f-\bar{f}$, which is 0 at $m=0$]

$T < T_c$, $m \neq 0$ gives minimum f [as well as $f-\bar{f}$]

(m=0 is a local maximum)

Ising Model

$$f-\bar{f} = -\bar{f} + \frac{Jz}{2}m^2 - kT\ln\left[2\cosh\left(\frac{Jz}{kT}m\right)\right]$$

for $B=0$

$(Jz = kT_c)$

$$= -\bar{f} + \frac{kT_c}{2}m^2 - kT\ln\left[2\cosh\left(\frac{T_c}{T}\cdot m\right)\right]$$

$$= \frac{kT_c}{2}m^2 - kT\ln\left[\cosh\left(\frac{T_c}{T}\cdot m\right)\right]$$

$$= \frac{kT_c}{2}m^2 - kT\ln\left[1 + \frac{1}{2}\left(\frac{T_c}{T}\right)^2 m^2 + \frac{1}{24}\left(\frac{T_c}{T}\right)^4 m^4\right]$$

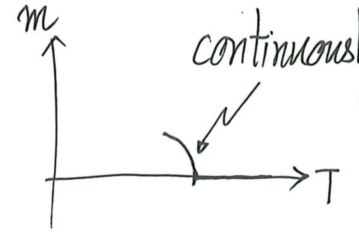
(look at $\cosh x$ for $x \ll 1$)

$$= \frac{kT_c}{2}m^2 - kT\cdot\frac{1}{2}\left(\frac{T_c}{T}\right)^2 m^2 + kT\cdot\frac{1}{12}\left(\frac{T_c}{T}\right)^4 m^4 \quad (23)$$

(Ex.) $\ln(1+x) \approx x - \frac{x^2}{2}$

$$\therefore \quad \underset{\substack{\uparrow \\ m^0 \\ \text{term}}}{f - \bar{f}} = \frac{k}{2}\frac{T_c}{T}\underbrace{(T-T_c)}_{\substack{\text{changes sign when} \\ T \text{ gets across } T_c}} \underset{\substack{\uparrow \\ m^2 \\ \text{term}}}{m^2} + \underbrace{\frac{1}{12} kT\left(\frac{T_c}{T}\right)^4}_{\text{positive}} \underset{\substack{\uparrow \\ m^4 \text{ term}}}{m^4} + (\text{higher powers} \sim m^6, \ldots)$$

gives



$$\text{OR} \quad f(m) = \bar{f} + \underbrace{a_2(T)}_{\substack{\sim a(T-T_c) \\ \uparrow \\ \text{changes sign}}} m^2 + \underset{\substack{\uparrow \\ a_4 > 0}}{a_4} m^4 \qquad (24) \quad (\text{for } B=0)$$

This is what mean-field theory for the Ising Model suggests.

And this is the empirical form of Landau's free energy in his <u>Landau Theory of continuous phase transitions</u>.

When there is an applied field B, we go back to Eq.(21) and repeat the steps

$$f(m) = \bar{f} + a_2(T)\, m^2 + a_4\, m^4 - (\text{constant})\, \underbrace{\underset{\substack{\uparrow\\ \text{order parameter}}}{m}\ \underset{\substack{\uparrow\\ \text{external field}}}{B}}_{\text{suggests the term in } f \text{ describing the coupling between order parameter and an external field}}$$

The effect is to drive the transition to become 1st order transition

I. Landau Theory of Continuous Phase Transitions.

Landau (1937)

- Introduced the idea of order parameter η [free from any specific problems]
  - ferromagnets : magnetisation
  - Superconductors : fraction of electrons becoming Cooper pairs (gap parameter)
  - Liquid crystals : Angle between director of molecule to alignment direction
  - Quasi-Crystals : Set of 5-fold symmetrical vectors

  Often given a problem, one needs to look for the proper order parameter
- Write free energy in powers of m, as $|m| \ll 1$ near critical point
- Powers of m reflect symmetry of system [Hamiltonian]

Then, Landau introduced (for $B=0$)

$$\boxed{f(\eta) = \underbrace{f_0}_{\sim m^0 \text{ term}} + \underbrace{a_2(T)}_{\sim a(T-T_c)\ \&\ \text{changes signs}} \eta^2 + \underbrace{a_4}_{a_4>0} \eta^4}^{+} \quad (25)$$

as a phenomenological (唯像) theory of critical phenomena

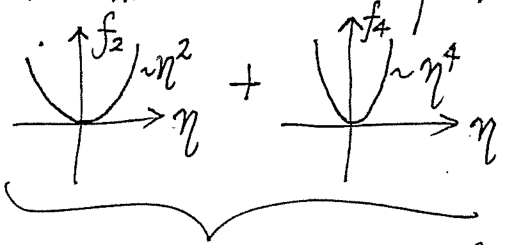
Ising case: Only up & down. The Hamiltonian has up/down symmetry. The m^2 and m^4 terms do not distinguish directions, thus they go with the symmetry of Hamiltonian. The $T>T_c$ paramagnetic phase also respects the symmetry. But the $T<T_c$ ferromagnetic phase has to pick a direction as it forms!

Big idea: Attached to critical phenomena is the idea of spontaneous symmetry breaking!

+ In Landau's Theory, η is the order parameter (not necessarily the magnetization). It can be a complex quantity, and η^2 means $|\eta|^2$, etc. This is the case in superfluidity and superconductivity.

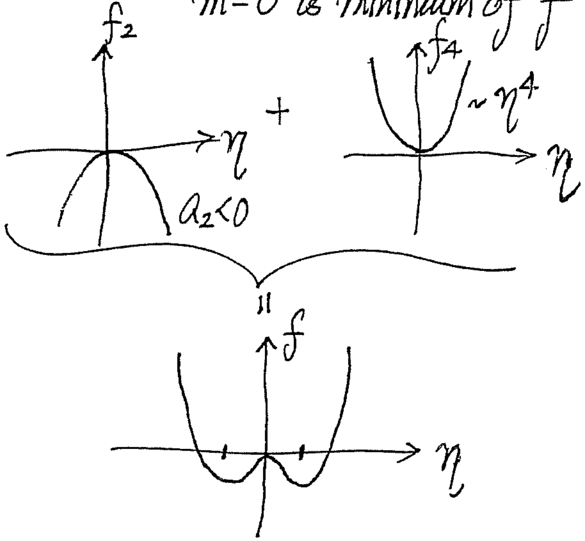
With $a_2(T) \sim (T-T_c)$ changing signs across T_c

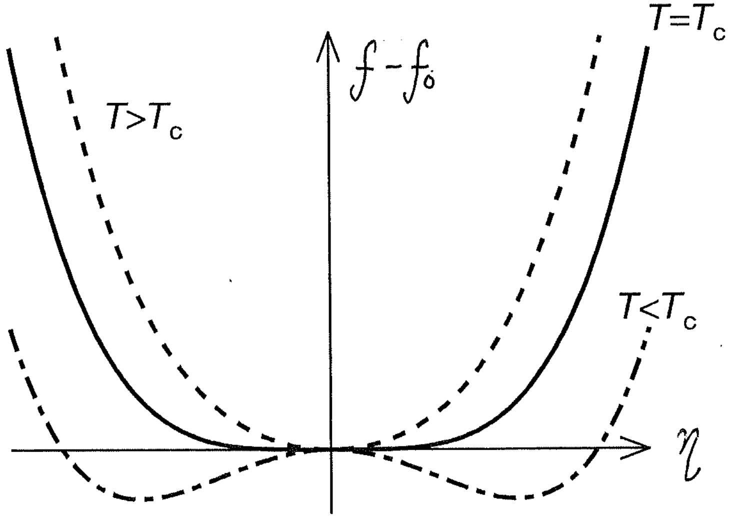
$T > T_c$: m^2 and m^4 terms are positive



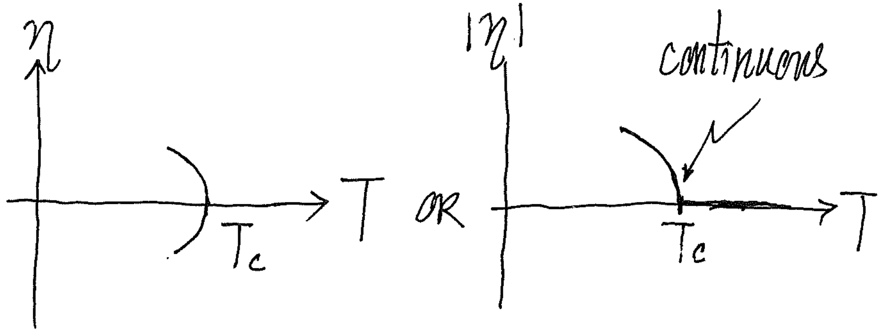
$m = 0$ is minimum of f

$T < T_c$:



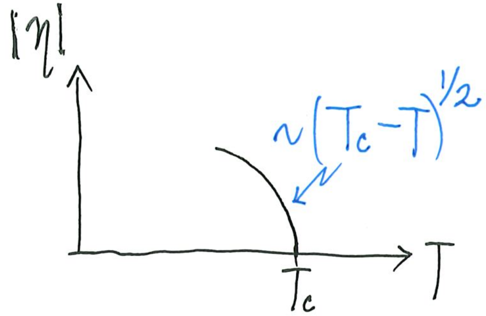


The two minima on either side of $m=0$ grow continuous from $\eta = 0$ as T becomes $T < T_c$.



Generally, $\dfrac{\partial f}{\partial \eta} = 0 \Rightarrow 2a_2(T)\,\eta + 4a_4\,\eta^3 = 0$

$$\Rightarrow \eta^2 = -\frac{a_2(T)}{2a_4} = \frac{a_0}{2a_4}(T_c - T), \quad \text{OR} \quad \underbrace{\eta = 0}_{\text{for } T > T_c}$$



$$\Rightarrow \eta = \pm\sqrt{\frac{a_0}{2a_4}}\,(T_c - T)^{1/2} \quad \text{for } T < T_c \qquad (26)$$

$\therefore \beta = 1/2$ (Landau Theory)

Substituting η back into $f(\eta)$, we obtain the value of the minimum of f (or $f - f_0$) as (for $T < T_c$)

$$f_{min} = f_0 - \underbrace{\frac{a_0^2}{4a_4}(T_c - T)^2}_{\text{"drops continuously" from } T = T_c \text{ and becomes lower and lower as } T < T_c} \qquad (27) \text{ (Ex.)}$$

From $f(\eta)$, one can study the entropy and heat capacity and their continuity (discontinuity) as T gets across T_c.

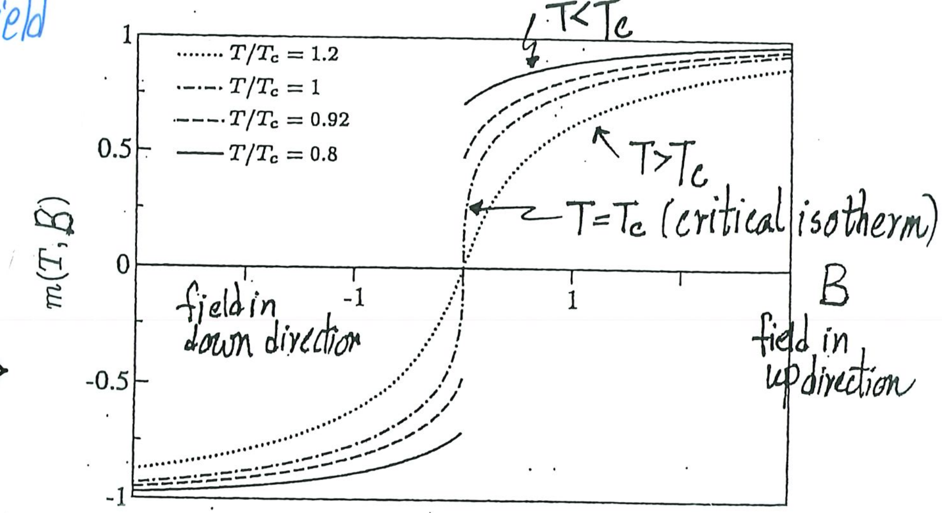
When there is an external field that can couple with the order parameter η,

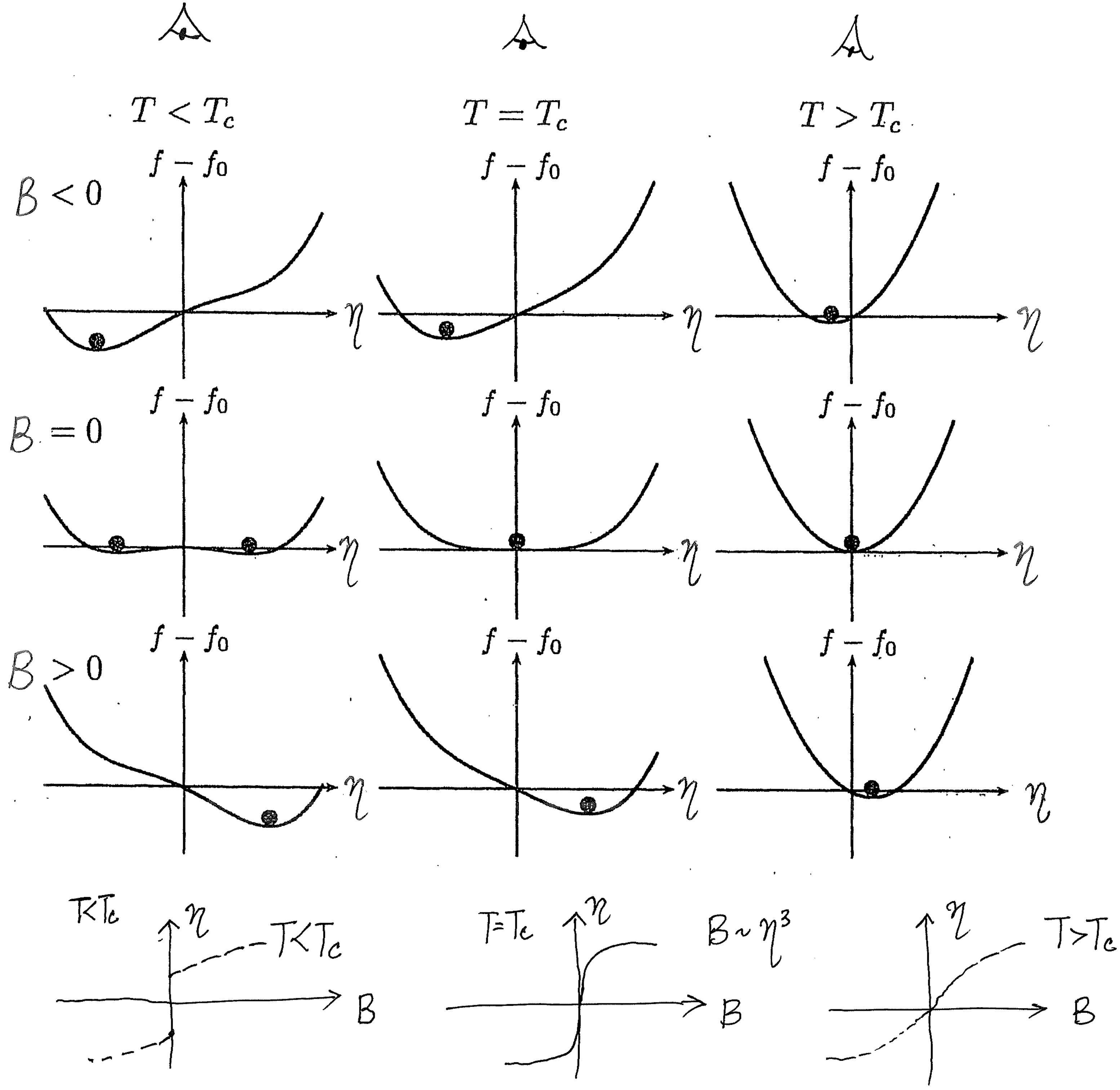
$$f(\eta) = f_0 \underbrace{- B\eta}_{\text{effect of an external field}} + a_2(T)\eta^2 + a_4\eta^4 \qquad (28)$$

We saw this in Ising Model →

(T<Tc, there is a jump from +m to −m)

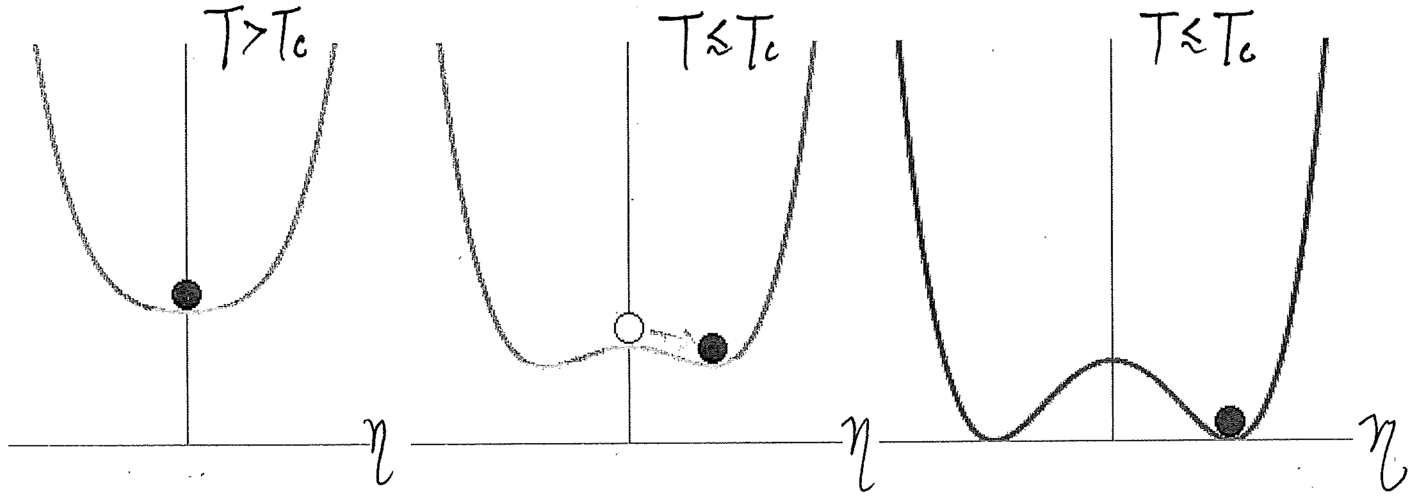
c.f. Δv is a jump in volume (vdW eq.)





T < Tc
T = Tc
T > Tc
B < 0
B = 0
B > 0
f − f0
η
T<Tc
T=Tc
B ~ η3
T>Tc
B

Back to $B=0$,



System needs to pick a direction (side)
In doing so, there is the notion of
what is the "up" side and what is the "down" side.
A particular direction is chosen spontaneously, and
the "up/down" symmetry is gone (broken).

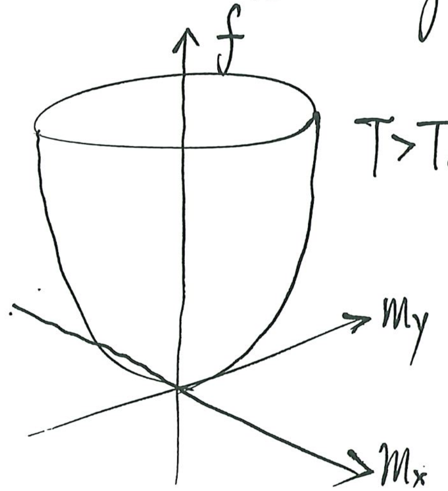
The idea is general! [Not only for Ising Model]

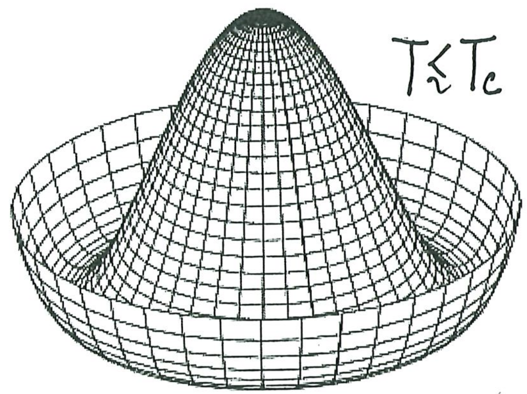
E.g. Each spin can point to <u>any direction</u> on a plane

(XY model)

$T > T_c$: Paramagnetic phase has "circular" symmetry †

$T < T_c$: System needs to select a direction





"shape of a Mexican hat"

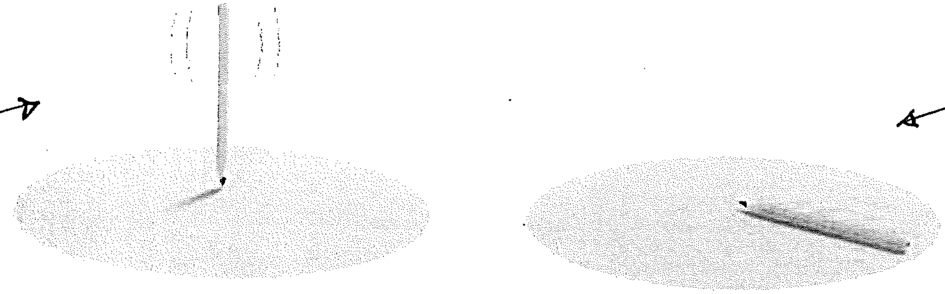
There is a ring of possible states with $|m| \neq 0$.
But system needs to take a direction.

† Same goes with problems with a complex scalar order parameter $\Delta = |\Delta| e^{i\phi}$, ϕ needs to take a value.

A usual analogy of this phenomenon is that of a fallen pencil.

All directions look the same

fallen pencil picks a direction



Spontaneous broken symmetry. The world of this pencil is completely symmetrical. All directions are exactly equal. But this symmetry is lost when the pencil falls over. Now only one direction holds. The symmetry that existed before is hidden behind the fallen pencil.

Marble on top of Mexican hat

Marble rolls down in a direction

All these phenomena come from a mathematical form:

$$f(\eta) = f_0 + a_2(T)\,\eta^2 + a_4\,\eta^4$$

or often written as:

$$f(\phi) = f_0 + a_2(T)\,\phi^2 + a_4\,\phi^4$$ where ϕ is the order parameter

Continuum (field)

- Spatial dependent $\eta(\vec{r})$

(not only up down spins, and $\vec{m}(\vec{r})$)

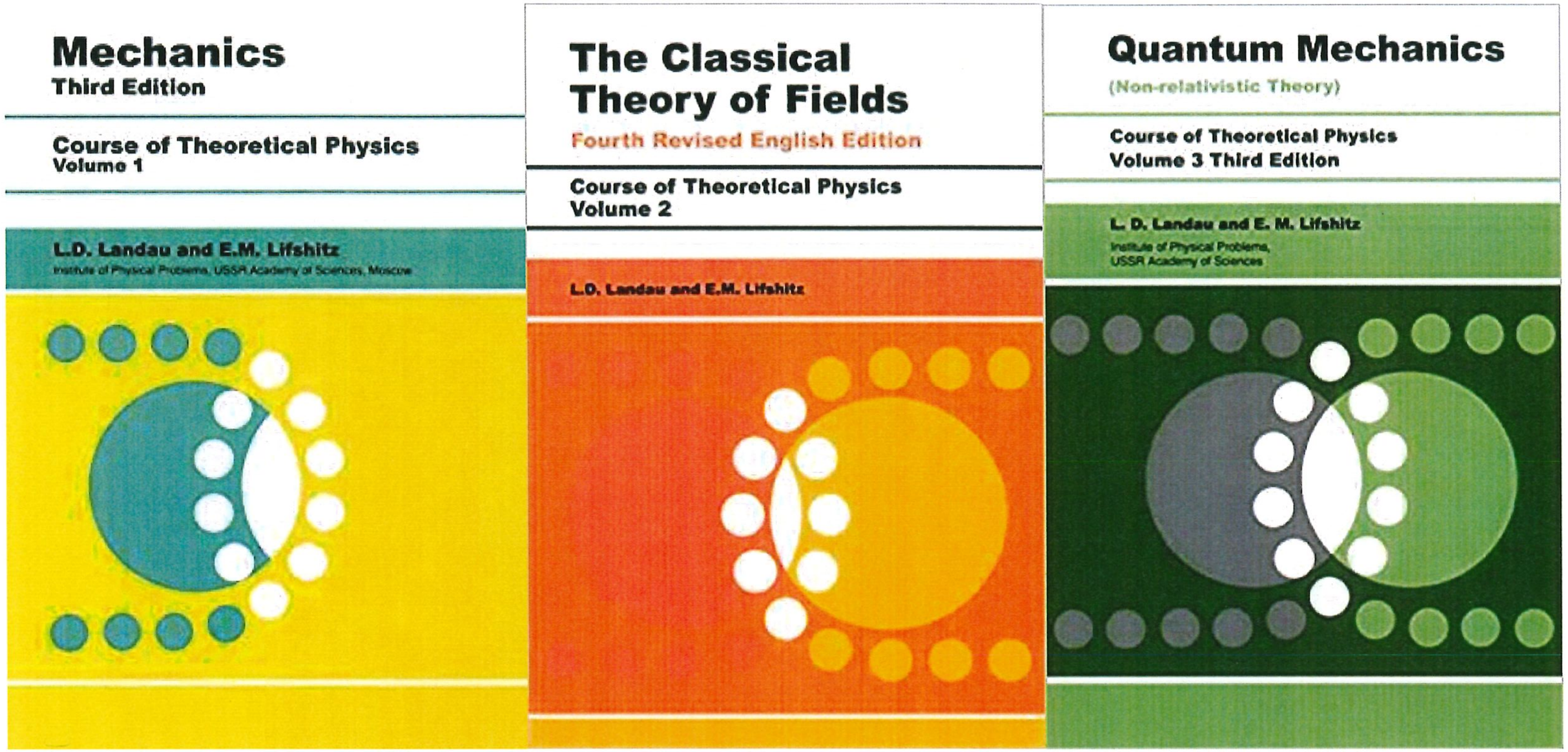
e.g. $\uparrow \nearrow \nearrow \nearrow \rightarrow \rightarrow \searrow \downarrow \downarrow \downarrow$

$\rightarrow$ a region that $\leftarrow$
spins(moments) switch from up to down
"domain wall" in magnetism

Landau Theory of Continuous Transitions can be generalized to the "Ginzburg - Landau Theory".

2003 Nobel Prize 1962 Nobel Prize

$$\mathcal{F} = \int d^3r\, f(\vec{r}) \quad \text{and} \quad f(\vec{r}) = a_2\,\eta^2(\vec{r}) + a_4\,\eta^4(\vec{r}) + G\underbrace{\left(\nabla\eta(\vec{r})\right)^2}_{\text{"gradient" (bending) energy}} \qquad (29)$$



Lev Landau (1908-1968)

- Top Physicist of 20th century
- Established Soviet Union's theoretical physics
- "Theoretical Minimum"

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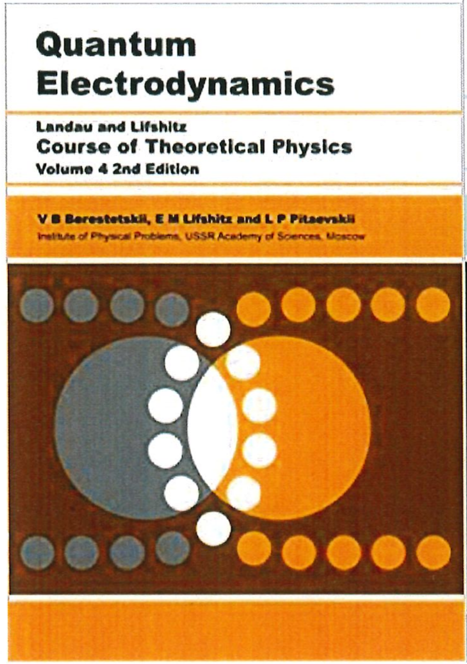
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V B Berestetskii, E M Lifshitz and L P Pitaevskii
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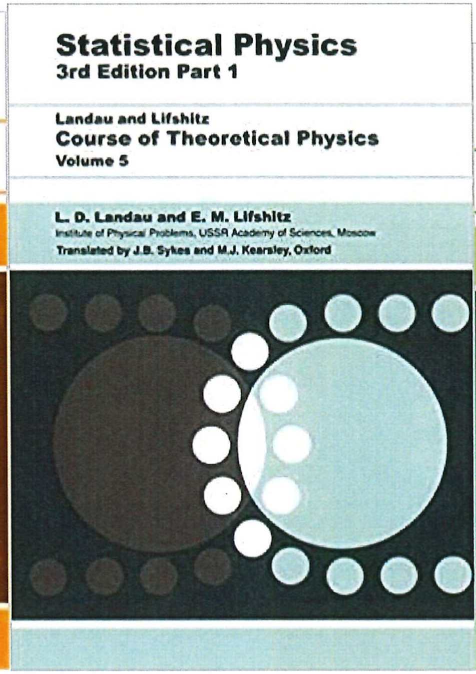
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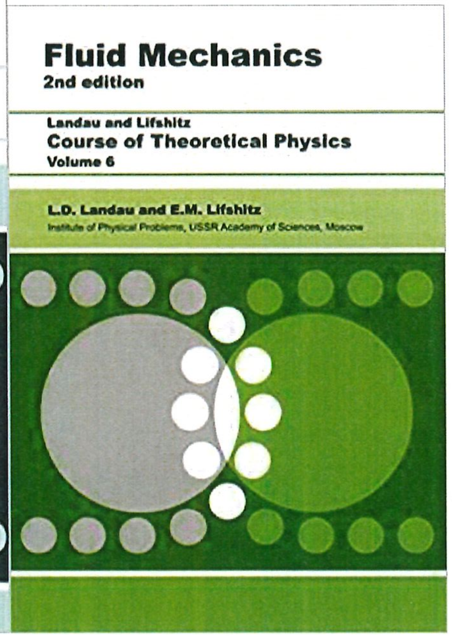
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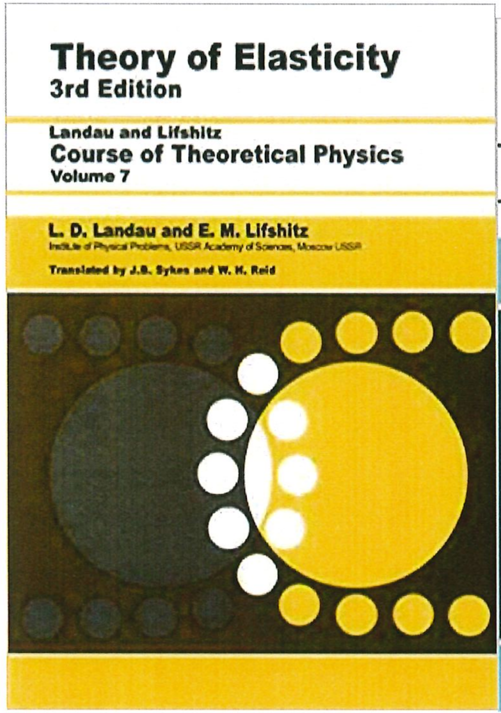
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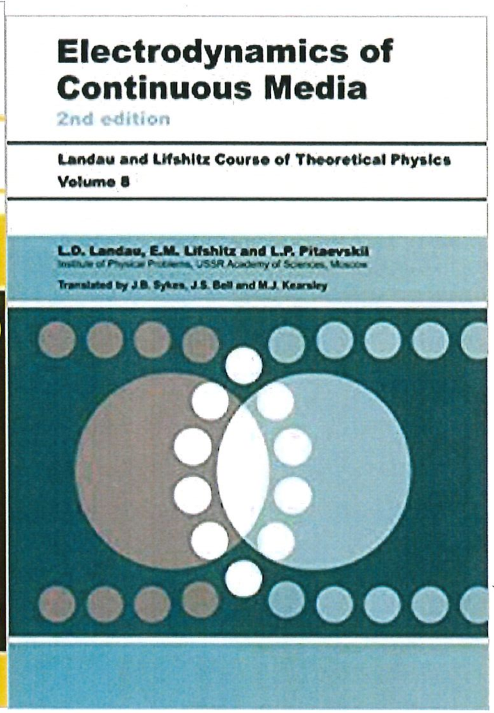
Electrodynamics of Continuous Media
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L.D. Landau, E.M. Lifshitz and L.P. Pitaevskii
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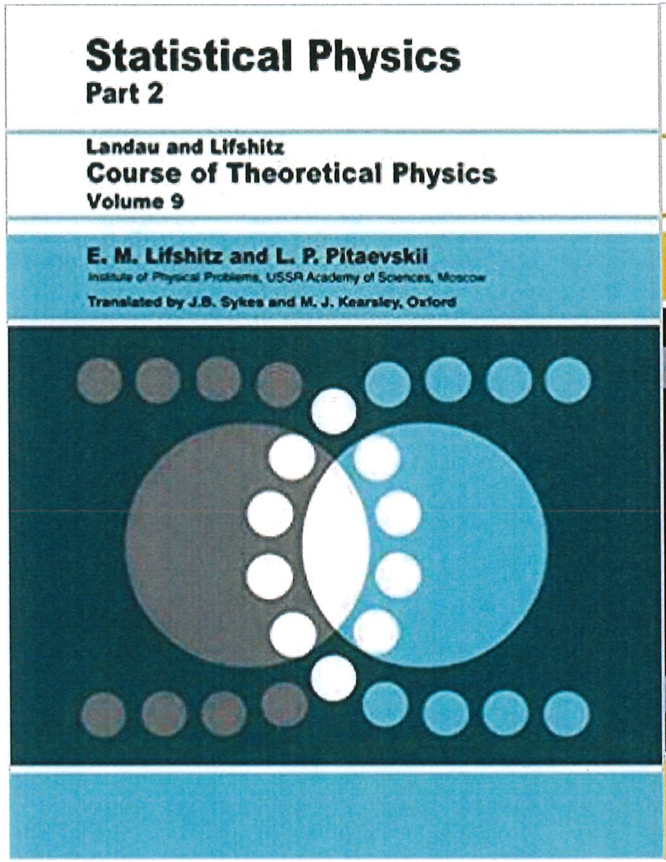
Statistical Physics
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Landau and Lifshitz
Course of Theoretical Physics
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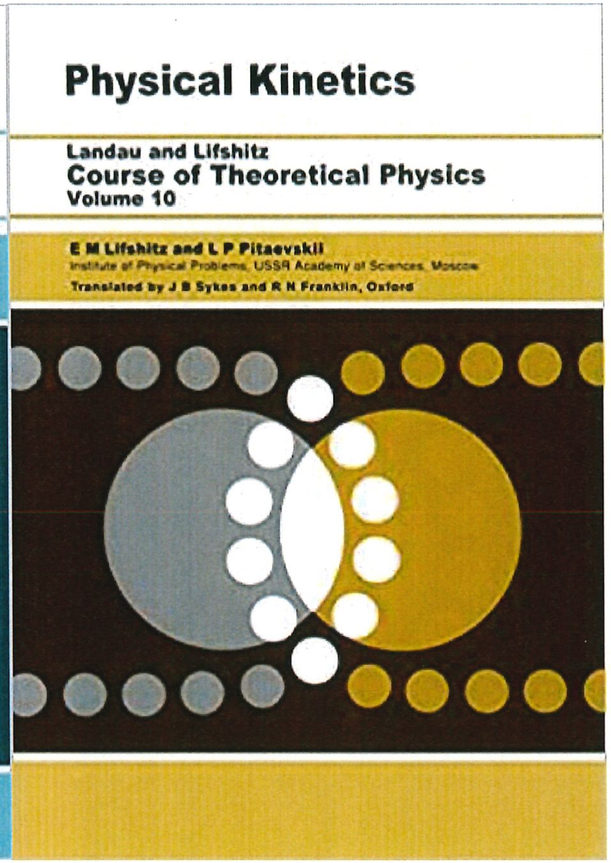
Physical Kinetics
Landau and Lifshitz
Course of Theoretical Physics
Volume 10
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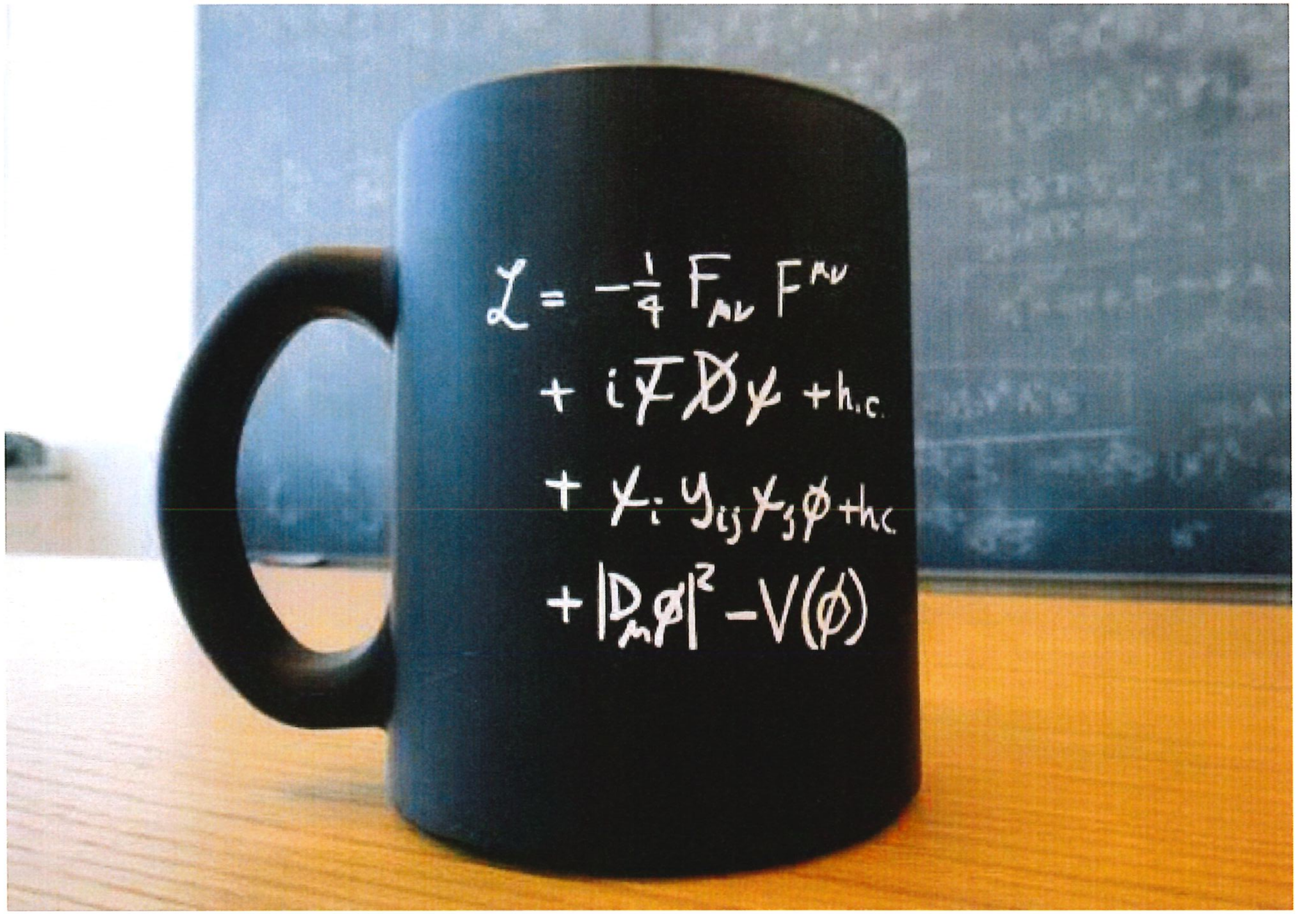
Institute of Physical Problems, USSR Academy of Sciences, Moscow
Translated by J B Sykes and R N Franklin, Oxford

The Standard Model



Product of CERN

$\mathcal{L}$ is the Lagrangian Density of the standard model
"$F_{\mu\nu} F^{\mu\nu}$" has all the particles (gauge bosons) responsible for EM, strong, weak forces;
"ψ and $\bar{\psi}$" have all the leptons and quarks.

As symmetry dictated the development of 20th century physics, the idea of spontaneous symmetry breaking played an important role in particle physics.+

$$
\begin{aligned}
L = & -\frac{1}{4}W_{\mu\nu}W^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}G_{\mu\nu}G^{\mu\nu} \\
& + \overline{\psi}_j \gamma^\mu (i\partial_\mu - g\tau_j \cdot W_\mu - g' Y_j B_\mu - g_s \mathbf{T}_j \cdot \mathbf{G}_\mu)\psi_j \\
& + |D_\mu \phi|^2 + \mu^2 |\phi|^2 - \lambda |\phi|^4 \\
& - (y_j \overline{\psi}_{jL} \phi \psi_{jR} + y_j' \overline{\psi}_{jL} \phi_c \psi_{jR} + \text{conjugate})
\end{aligned}
$$

Lagrangian Density of the Standard Model (long form)

Higgs Mechanism

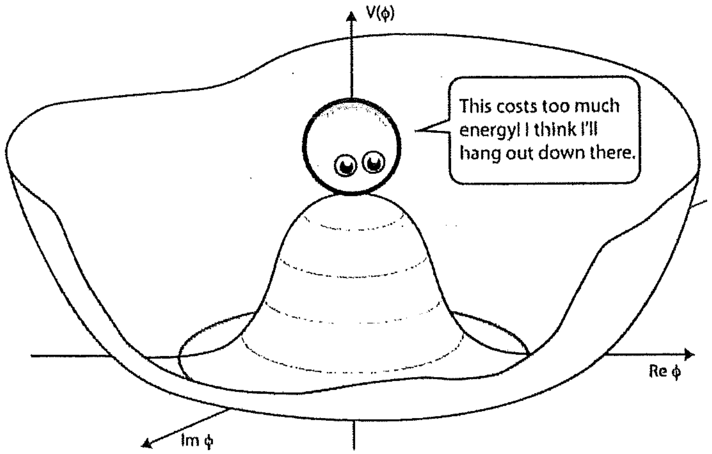
$$\Big(\underbrace{|D_\mu \phi|^2}_{\text{kinetic energy term (like } (\nabla\phi)^2)} - \big[\underbrace{-\mu^2 |\phi|^2 + \lambda |\phi|^4}_{\text{Mexican hat shape}} \big] \Big)$$

ϕ is the Higgs field

kinetic energy term (like $(\nabla \phi)^2$)

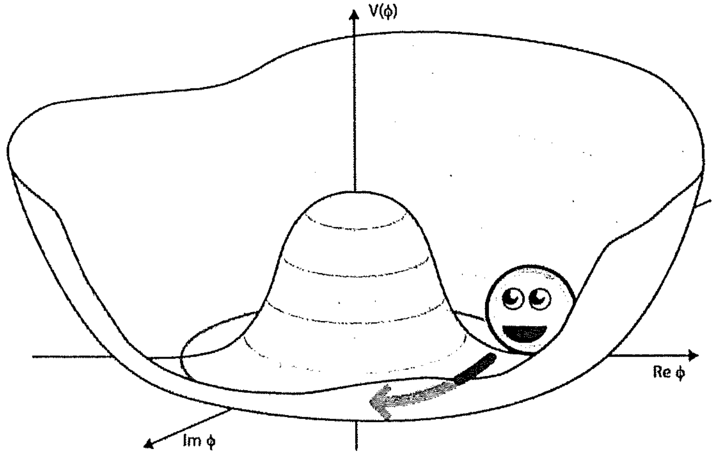
Mexican hat shape } so ϕ picks a direction (spontaneous symmetry breaking) and takes on a certain value.

+ Nobel Prize (2008) to Nambu, Kobayashi, Maskawa for their work on spontaneous symmetry breaking in subatomic physics. The Higgs mechanism (Nobel Prize 2013) is also related to SSB.

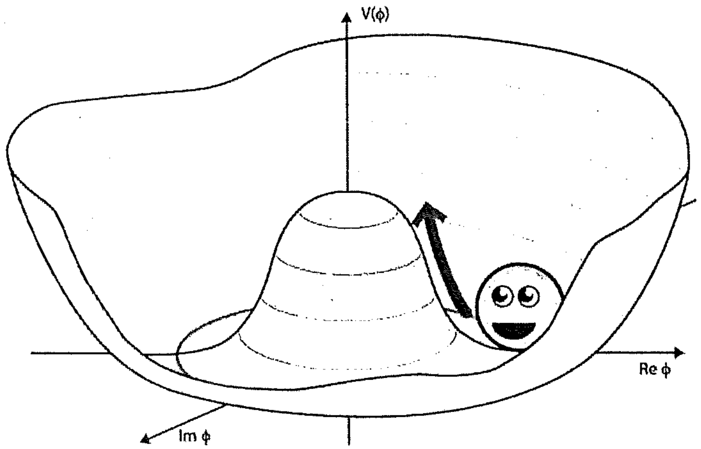


Source: http://cph-theory.persiangig.com/90.11.26-3.htm

See also Nobel Prize Announcements in 2008 and 2013.



Symmetry breaking
Higgs field picks a direction [real value]



Low-energy excitation

- massive
- massless

Refs: For students who want to learn more on phase transitions and critical phenomena, see

- M. Gitterman, "Phase Transitions: Modern Applications" (World Scientific)
- J.M. Yeomans, "Statistical Mechanics of Phase Transitions" (Clarendon Press)
- K. Christensen & N.R. Moloney, "Complexity and Criticality" (Imperial College Press)
- D. Khomskii, "Basic Aspects of the Quantum Theory of Solids" (Cambridge Univ. Press), Ch. 2