Mean-field approximation for Ising model

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0 Mean-field approximation (MFA)

- a simple approach to many-particle interacting systems
- a reduction to an effective one-particle problem
- both for classical and quantum systems
- reliability in solid-state physics: depending on dimension (1D - not valid, 3D - semiquantitative validity, 2D - depends on details of the model/system)
- recently extended to a dynamical mean-field theory

in this lecture:

¶ justification of the MFA from a variational principle (Peierls/Feynman/Bogolyubov inequality)

¶ MFA for the classical Ising model of magnetism

1 Peierls-Feynman inequality

• for two Hamiltonians H and H_0 that differ by a quantity $V \equiv H - H_0$ and for the corresponding free energies F and F_0 (at a given temperature T), the following inequality holds:

$$F \leq F_0 + \langle V \rangle_0 = F_0 + \langle H - H_0 \rangle_0 \,, \tag{1}$$

where $\langle \dots \rangle_0$ denotes the thermodynamic average with respect to the unperturbed Hamiltonian H_0

• practical importance of the inequality:
H is usually the Hamiltonian of a real system, i.e., it is difficult for an exact treatment, while H_0 is the Hamiltonian of a simpler model system that can be treated exactly including an evaluation of the r.h.s. of Eq. (1).

H_0 depends on unknown parameters a_i $(i = 1, 2, \ldots)$, so that the r.h.s. of Eq. (1) becomes a function of these parameters,

$$F_0 + \langle H - H_0 \rangle_0 \;\equiv\; \Phi(\{a_i\})\,.$$

The values of $\{a_i\}$ can be found by minimization of the function $\Phi(\{a_i\})$, which yields an approximate value of the free energy F as a function of the temperature (and of other parameters of the Hamiltonian H, e.g., external fields):

$$F_{\rm appr} \;=\; \min_{\{a_i\}} \Phi(\{a_i\})\,.$$

This approximate free energy leads then to other physical quantities (entropy, energy, specific heat, magnetization, $\ldots$).

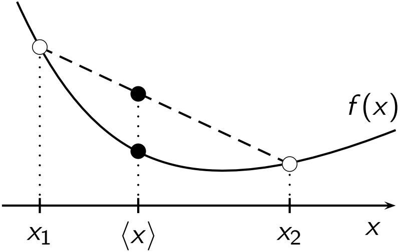
• *Proof of the inequality* (for the classical case):

$$\begin{aligned}\exp(-\beta F) &= \int \exp(-\beta H)\,\mathrm{d}\Gamma\,, \\ \exp(-\beta F_0) &= \int \exp(-\beta H_0)\,\mathrm{d}\Gamma\,, \\ \langle A\rangle_0 &= \frac{\int A\exp(-\beta H_0)\,\mathrm{d}\Gamma}{\int \exp(-\beta H_0)\,\mathrm{d}\Gamma}\,,\end{aligned}$$

where $\beta = 1/(k_B T)$, $\mathrm{d}\Gamma \equiv \mathrm{d}p\,\mathrm{d}q$, and $A = A(p,q)$ denotes an arbitrary quantity. For $A = \exp(-\beta V)$ it yields:

$$\begin{aligned}\exp(-\beta F) &= \int \exp(-\beta H_0)\exp(-\beta V)\,\mathrm{d}\Gamma \\ &= \exp(-\beta F_0)\langle\exp(-\beta V)\rangle_0\,.\end{aligned}$$

The real function $V \mapsto \exp(-\beta V)$ is convex, which means that for any average $\langle \dots \rangle$ with positive weights, a general relation $\langle \exp(-\beta V) \rangle \geq \exp(-\beta \langle V \rangle)$ is valid.



$f(x)$ – convex:

$$f''(x) \geq 0$$

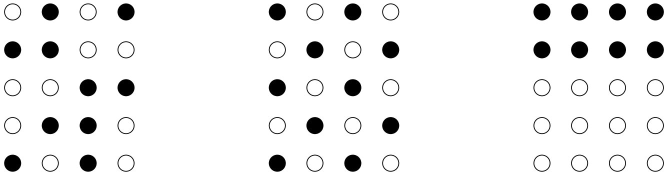
$$\langle f(x) \rangle \geq f(\langle x \rangle)$$

For the thermodynamic average $\langle \dots \rangle_0$, one gets

$$\begin{aligned} \langle \exp(-\beta V) \rangle_0 &\geq \exp(-\beta \langle V \rangle_0) \\ \Longrightarrow \quad \exp(-\beta F) &\geq \exp(-\beta F_0) \exp(-\beta \langle V \rangle_0), \end{aligned}$$

which is equivalent to Eq. (1).
For the quantum case: R. P. Feynman: Statistical Mechanics, or S. V. Tyablikov: Methods of Quantum Theory of Magnetism.

2 Ising model of magnetism



magnetism: $\Uparrow$, $\Downarrow$ (local spins)

binary alloys: A, B (atomic species)

a simple classical model to study:

- phase transitions
- appearance of complex orders

• the Ising Hamiltonian is defined as

$$H = -\frac{1}{2}\sum_{mn} J_{mn} s_m s_n - \sum_m b_m s_m , \qquad (2)$$

where m, n – lattice sites, $s_m \in \{+1, -1\}$ – the direction of a classical local moment (spin) at the m-th site, the exchange integrals J_{mn} – pair interaction of the local spins ($J_{mm} = 0$, $J_{mn} = J_{nm}$), and b_m – local magnetic fields interacting with the individual local spins

• the model Hamiltonian is taken in a form

$$H_0 = -\sum_m a_m s_m , \qquad (3)$$

where a_m denote (yet unspecified) local magnetic fields. This Hamiltonian does not contain interaction among the spins and it is easy to deal with.

- the quantities entering the r.h.s. of Eq. (1) are equal to

$$\begin{aligned}
Z_0 &= \sum_{\{s_m\}} \exp(-\beta H_0) = \sum_{\{s_m\}} \exp\left(\beta \sum_m a_m s_m\right) \\
&= \prod_m z_m \,, \qquad z_m = \sum_{s_m=-1}^{+1} \exp(\beta a_m s_m) = 2\cosh(\beta a_m)\,, \\
F_0 &= -\beta^{-1} \ln Z_0 = -\beta^{-1} \sum_m \ln[2\cosh(\beta a_m)]\,, \\
\langle H_0 \rangle_0 &= -\sum_m a_m \langle s_m \rangle_0 \,, \\
\langle s_m \rangle_0 &= z_m^{-1} \sum_{s_m=-1}^{+1} s_m \exp(\beta a_m s_m) = \tanh(\beta a_m)\,, \\
\langle H \rangle_0 &= -\frac{1}{2} \sum_{mn} J_{mn} \langle s_m \rangle_0 \langle s_n \rangle_0 - \sum_m b_m \langle s_m \rangle_0 \,,
\end{aligned}$$

where the relation $\langle s_m s_n \rangle_0 = \langle s_m \rangle_0 \langle s_n \rangle_0$ was used that is valid for the non-interacting Hamiltonian H_0.

The function to be minimized [$\equiv$ r.h.s. of Eq. (1)] thus reads:

$$\begin{aligned}\Phi(\{a_i\}) \;=\; &-\frac{1}{2}\sum_{mn} J_{mn} \tanh(\beta a_m) \tanh(\beta a_n) \\ &- \sum_m b_m \tanh(\beta a_m) \,-\, \beta^{-1} \sum_m \ln[2\cosh(\beta a_m)] \\ &+ \sum_m a_m \tanh(\beta a_m)\,. \end{aligned} \qquad (4)$$

The usual conditions of stationarity ($\partial\Phi/\partial a_j = 0$) lead to equations:

$$
\begin{aligned}
&- \sum_n J_{jn} \frac{\beta}{\cosh^2(\beta a_j)} \tanh(\beta a_n) \; - \; b_j \frac{\beta}{\cosh^2(\beta a_j)} \\
&- \beta^{-1} \frac{\sinh(\beta a_j)}{\cosh(\beta a_j)} \beta \; + \; \tanh(\beta a_j) \; + \; a_j \frac{\beta}{\cosh^2(\beta a_j)} \;\; = \;\; 0 \, .
\end{aligned}
$$

The 3rd and 4th terms on the l.h.s. cancel mutually and the resulting equations are:

$$
a_j \; = \; b_j \; + \; \sum_n J_{jn} \tanh(\beta a_n) \, , \tag{5}
$$

which represents a set of coupled non-linear equations for the set of unknown variables $\{a_i\}$.

• with abbreviation $\bar{s}_n \equiv \langle s_n \rangle_0$, the previous equations are usually recast as

$$\bar{s}_j = \tanh(\beta a_j)\,, \qquad \underbrace{a_j}_{(*)} = \underbrace{b_j}_{(**)} + \underbrace{\sum_n J_{jn}\bar{s}_n}_{(***)}\,, \tag{6}$$

which has a clear physical interpretation:

the average value of the spin on a given site is given by the effective field (*) which is equal to the sum of the applied (external) field (**) and a term depending on the average moments on the surrounding sites, the so-called Weiss (molecular) field (***)

¶ the equations (5, 6) define the mean-field approximation (MFA) to the original Ising Hamiltonian

¶ MFA for alloys: Bragg-Williams approximation

• a note to the meaning of $\bar{s}_n \equiv \langle s_n \rangle_0$ $[= \tanh(\beta a_n)]$:
the Ising Hamiltonian H, Eq. (2), leads to exact relations

$$\frac{\partial H}{\partial b_n} = -\, s_n \qquad \Longrightarrow \qquad \langle s_n \rangle = -\frac{\partial F}{\partial b_n} .$$

Within the MFA, the exact free energy F is replaced by $F_{MFA} = \min_{\{a\}} \Phi(\{a_i\})$, which leads to

$$\langle s_n \rangle_{MFA} = -\frac{\partial F_{MFA}}{\partial b_n} = \underbrace{\langle s_n \rangle_0}_{(*)} - \sum_j \frac{\partial \Phi}{\partial a_j} \frac{\partial a_j}{\partial b_n} = \langle s_n \rangle_0 = \bar{s}_n ,$$

where the term (*) corresponds to the explicit dependence of $\Phi(\{a_i\})$ on the b_n and where the condition of stationarity $(\partial \Phi / \partial a_j = 0)$ was employed.
This means that the quantity $\langle s_n \rangle_0 \equiv \bar{s}_n$ can really be identified with the MFA-average of the n-th spin.

• a note to the value of $\langle s_m s_n \rangle$ within the MFA:
in a complete analogy (by taking partial derivatives with respect to the exchange integrals J_{mn}), one can prove for $m \neq n$ that

$$\langle s_m s_n \rangle_{MFA} = \langle s_m \rangle_0 \langle s_n \rangle_0 = \bar{s}_m \bar{s}_n \, , \qquad (7)$$

which means that correlations between two different spins are neglected within the MFA

• a note on magnitudes of the molecular fields:
for typical magnets based on $3d$ transition metals (Mn, Fe, Co, Ni), the Weiss molecular fields can be ~ 100 T, i.e., much stronger than usual applied fields (not exceeding ~ 10 T)

3 Ferromagnetism

• let us consider a simple (Bravais) lattice with all sites equivalent and let us abbreviate

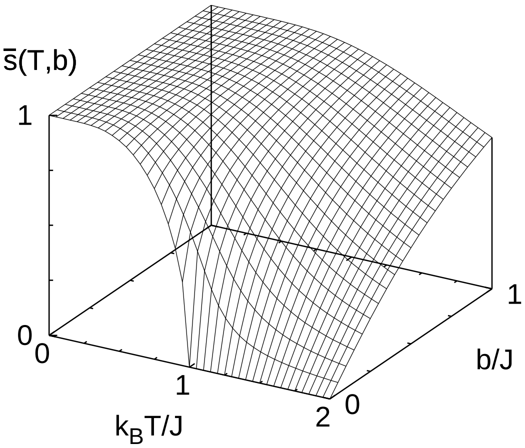
$$b_m = b\,, \quad a_m = a\,, \quad \langle s_m \rangle_0 = \bar{s}\,, \quad \sum_n J_{mn} = \mathcal{J}\,,$$

then the MFA equations (5, 6) reduce to

$$\bar{s} = \tanh(\beta a)\,, \quad a = b + \mathcal{J}\bar{s}\,, \quad \bar{s} = \tanh[\beta(b + \mathcal{J}\bar{s})]\,. \quad (8)$$

For a ferromagnet, most of the pair interactions J_{mn} are non-negative and we assume $\mathcal{J} > 0$.

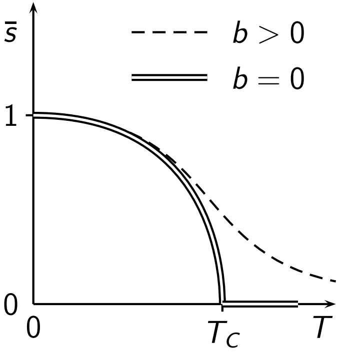
• solution to Eq. (8) $\Longrightarrow$ the average spin $\bar{s}$ as a function of the temperature T and the external field b: $\bar{s} = \bar{s}(T, b)$



The solution $\bar{s} = \bar{s}(T, b)$ of Eq. (8) vs. a dimensionless temperature $(k_B T/\mathcal{J})$ and a dimensionless field $(b/\mathcal{J})$ [for $b \leq 0$ one employs $\bar{s}(T, b) = -\bar{s}(T, -b)$].

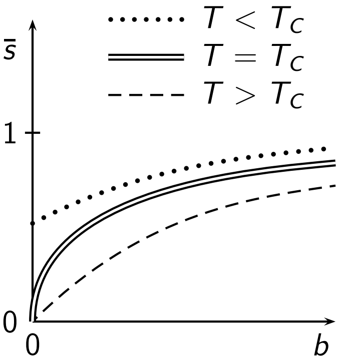
- $\mathcal{J}/k_B \equiv T_C$ is the Curie temperature

$\bar{s}(T,b)$ for fixed b:



$\bar{s}(T,0)$ – spontaneous magnetization

$\bar{s}(T,b)$ for fixed T:



$\bar{s}(T_C,b)$ – critical isotherm

3.1 Solution for high temperatures

• for small external fields, $b \to 0$, and high temperatures T, Eq. (8) has a unique solution that follows from $\tanh(x) \approx x$ for $|x| \ll 1$:

$$\bar{s} = \beta(b + \mathcal{J}\bar{s}), \qquad \bar{s} = \frac{\beta b}{1 - \beta\mathcal{J}} = \frac{b}{k_B T - \mathcal{J}}. \tag{9}$$

This can be written in a form of the Curie-Weiss law

$$\bar{s}(T, b) = \chi(T) b, \quad \chi(T) = \frac{1}{k_B T - \mathcal{J}} = \frac{C}{T - T_C}, \tag{10}$$

where $\chi(T)$ denotes the susceptibility, $C = 1/k_B$, and

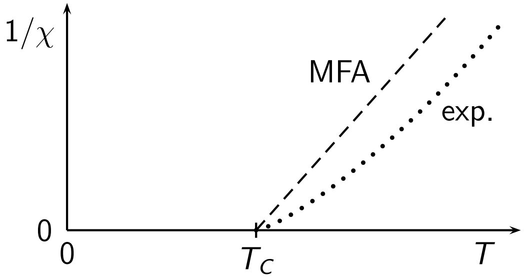
$$T_C = \mathcal{J}/k_B \tag{11}$$

is the Curie temperature in the MFA.

• the experimentally found susceptibilities for $T \to T_C^+$ follow a relation (critical behavior):

$$\chi(T) \sim (T - T_C)^{-\gamma} , \qquad (12)$$

where γ is one of the so-called critical exponents;
the value of $\gamma = 1$, Eq. (10), is typical for the MFA while experimental values for ferromagnetic metals (Fe, Co, Ni, Gd) lie in the range $1.2 < \gamma < 1.33$



3.2 Solution for low temperatures

• for low temperatures ($T < T_C$, $\beta\mathcal{J} > 1$), a non-zero solution $\bar{s}$ exists even for vanishing external field ($b = 0$):

$$\bar{s} = \tanh(\beta\mathcal{J}\bar{s}) \, , \tag{13}$$

which defines the spontaneous magnetization

3.2.1 Temperatures near the Curie temperature

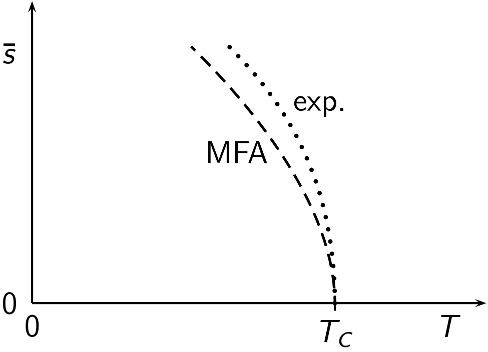
• for $T \to T_C^-$, the non-trivial solution $\bar{s} \to 0$ and one can use $\tanh(x) \approx x - \frac{1}{3}x^3$ for $|x| \ll 1$ in Eq. (13), which yields:

$$\bar{s}(T) \sim (T_C - T)^{1/2} \, , \tag{14}$$

whereas the critical behavior encountered in experiment and in more sophisticated theories is

$$\bar{s}(T) \;\sim\; (T_C - T)^{\beta}\,, \tag{15}$$

where β [to be distinguished from $\beta = 1/(k_B T)$!] is another critical exponent; its MFA value $\beta = 1/2$ exceeds measured values around $\beta \approx 0.35$



- a comparison of MFA with more sophisticated approaches (for 1st nearest-neighbor pair interactions J_{mn}):
  - 1D - exact treatment simple $\Longrightarrow$ no phase transition
  - 2D - exact treatment possible (L. Onsager)
  - 3D - Monte Carlo simulations

system	T_C / T_C^{MFA}	β
1D chain	–	–
2D square lattice	0.567	0.125
3D sc lattice	0.752	0.326
3D fcc lattice	0.816	0.326

¶ MFA overestimates both T_C and β $(\beta^{MFA} = 0.5)$

3.2.2 Temperatures close to zero

• for $T \to 0^+$, the non-trivial solution $\bar{s} \to 1$, and one can employ $\tanh(x) \approx 1 - 2\exp(-2x)$ for $x \gg 1$ in Eq. (13), which yields:

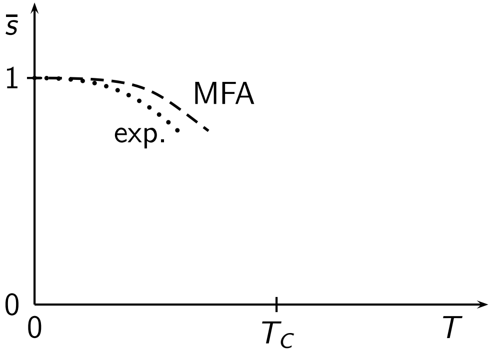
$$\bar{s}(T) \;=\; 1 - 2\exp\left(-\frac{2\mathcal{J}}{k_B T}\right) \,, \tag{16}$$

i.e., the finite temperature $T > 0$ causes a very slow initial decrease from the saturated value $\bar{s} = 1$ at $T = 0$

• interpretation of Eq. (16):
local spin reversals $(s_m = +1 \;\to\; s_m = -1)$
accompanied by an energy increase $2\mathcal{J}$
[with the Boltzmann probability $\exp(-\beta\, 2\mathcal{J})$]

• experiment (for cubic ferromagnets Fe and Ni) yields
a faster decrease: $\bar{s}(T) = 1 - AT^{3/2}$ – the Bloch 3/2-law

• origin of the Bloch law: Heisenberg model (instead of Ising), collective excitations (magnons), quantum statistics



3.2.3 Susceptibility

• the (differential) susceptibility in presence of spontaneous non-zero magnetization is defined as

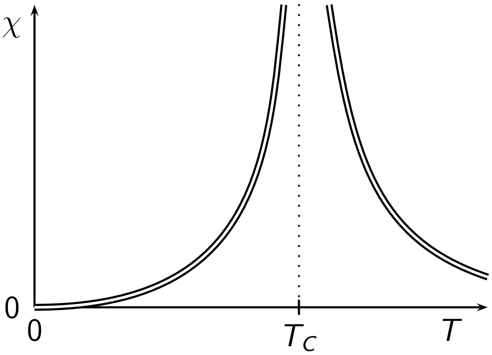
$$\chi(T) = \frac{\partial \bar{s}(T, b=0)}{\partial b}$$

and the partial derivative of $\bar{s} = \tanh[\beta(b + \mathcal{J}\bar{s})]$ leads to

$$\chi = \frac{\beta(1+\mathcal{J}\chi)}{\cosh^2(\beta\mathcal{J}\bar{s})}, \qquad \chi = \frac{\beta}{\cosh^2(\beta\mathcal{J}\bar{s}) - \beta\mathcal{J}},$$

$$\chi(T) \approx \frac{4}{k_B T}\exp\left(-\frac{2\mathcal{J}}{k_B T}\right) \qquad \text{for } T \to 0^+,$$

$$\chi(T) \approx \frac{1}{2k_B(T_C - T)} \qquad \text{for } T \to T_C^- \qquad (17)$$


χ
0
0
T_C
T

3.3 Critical isotherm

• for $T = T_C$ and for small external fields, $b \to 0^+$,
the value of $\bar{s}$ is obtained by solving $\bar{s} = \tanh[\beta(b + \mathcal{J}\bar{s})]$
with the use of $\tanh(x) \approx x - \frac{1}{3}x^3$ for $|x| \ll 1$;
with $\beta_C = (k_B T_C)^{-1} = \mathcal{J}^{-1}$ we get:

$$0 \;=\; \beta_C b - \frac{1}{3}(\beta_C b + \bar{s})^3 \,, \qquad \bar{s}(b) \;\approx\; \left(\frac{3b}{\mathcal{J}}\right)^{1/3} . \qquad (18)$$

This is another example of the critical behavior, namely

$$\bar{s}(b) \;\sim\; b^{1/\delta} \,, \qquad (19)$$

where the critical exponent $\delta = 3$ in the MFA
while its measured values lie around $\delta \approx 4$.

• the critical behavior in the MFA, Eqs. (10, 14, 17, 18), differs quantitatively from experimental behavior; however, both the measured and the MFA critical exponents ($\beta = 1/2, \;\; \gamma = 1, \;\; \delta = 3$) satisfy a rule

$$\delta \;=\; 1 + \frac{\gamma}{\beta}\,, \tag{20}$$

that follows from a 'scaling law' Ansatz

3.4 Energy, entropy, and specific heat

• the function to be minimized, Eq. (4), per one site of the ferromagnet is

$$\Phi_1(a) = -\frac{\mathcal{J}}{2}\tanh^2(\beta a) - b\tanh(\beta a) - k_B T\ \ln[2\cosh(\beta a)] + a\tanh(\beta a) \qquad (21)$$

• by employing the relation $\bar{s} = \tanh(\beta a)$, one can prove

$$a = \frac{1}{2\beta}\ln\frac{1+\bar{s}}{1-\bar{s}}\,, \qquad \cosh(\beta a) = \left(1-\bar{s}^2\right)^{-1/2}\,,$$

which can be substituted into $\Phi_1(a)$, Eq. (21).
This leads to the MFA-free energy per one site as a function of temperature and external field:

$$F_1(T,b) \; = \; -\frac{\mathcal{J}}{2}\,\bar{s}^2 \; - \; b\bar{s}$$
$$+\,k_B T \left(\frac{1+\bar{s}}{2} \ln \frac{1+\bar{s}}{2} \; + \; \frac{1-\bar{s}}{2} \ln \frac{1-\bar{s}}{2} \right) , \qquad (22)$$

where $\bar{s}$ depends implicitly on T and b due to the condition of stationarity: $\bar{s} = \tanh[\beta(b + \mathcal{J}\bar{s})]$.

• the internal energy per one site can be obtained from the average of the Hamiltonian H, Eq. (2), with the neglect of correlations in the MFA, Eq. (7) $[\ \langle s_m s_n \rangle \approx \bar{s}_m \bar{s}_n\ ]$:

$$U_1(T,b) \; = \; -\frac{\mathcal{J}}{2}\,\bar{s}^2 \; - \; b\bar{s} \qquad (23)$$

• the entropy per one site is now given by $(F_1 = U_1 - TS_1)$:

$$S_1(T,b) = -k_B \left(\frac{1+\bar{s}}{2} \ln \frac{1+\bar{s}}{2} + \frac{1-\bar{s}}{2} \ln \frac{1-\bar{s}}{2} \right), \quad (24)$$

which has a clear interpretation in terms of two probabilities $p_{\pm} = (1 \pm \bar{s})/2$ corresponding to the average spin $\bar{s}$

• the specific heat per one site (at a constant field b) equals

$$C_1(T,b) = \frac{\partial U_1(T,b)}{\partial T} = -\frac{\mathcal{J}}{2} \frac{\partial \bar{s}^2}{\partial T} - b \frac{\partial \bar{s}}{\partial T} \quad (25)$$

• at zero field $(b = 0)$ and for temperatures above the T_C:
$\bar{s} = 0 \implies S_1(T,0) = k_B \ln 2, \; U_1(T,0) = 0, \; C_1(T,0) = 0;$

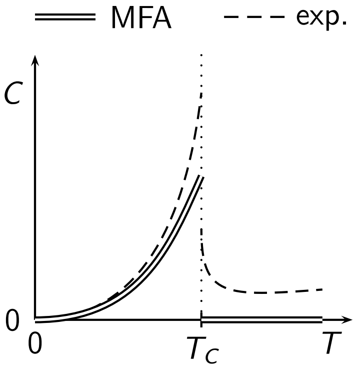
for temperatures slightly below the T_C:
$\bar{s}^2 \sim (T_C - T) \implies F_1(T,0),\; U_1(T,0),\; S_1(T,0)$ are continuous at $T = T_C$, whereas the specific heat $C_1(T,0)$ exhibits a discontinuity:

$$\lim_{T \to T_C^-} C_1(T,0) = \frac{3}{2}\, k_B \,,$$

$$\lim_{T \to T_C^+} C_1(T,0) = 0 \,, \quad (26)$$

$\implies$ the phase transition is of the second order

- experiment: 'lambda' point



3.5 MFA and the Landau theory of phase transitions

• the Landau theory of the 2nd-order phase transitions is based on a phenomenological free energy as a function of the order parameter $\bar{s}$ in the form of a 4th-degree polynomial:

$$\Psi_L(\bar{s}) = \phi(T) - b\bar{s} + c_2(T - T_C)\bar{s}^2 + c_4\bar{s}^4 , \qquad (27)$$

where: $\phi(T)$ – free energy of the paramagnetic phase,
c_2, c_4 – positive constants, T – temperature,
b – external field, T_C – the Curie temperature

- term $-b\bar{s} \equiv$ magnetic field $\times$ magnetic moment
- terms $()\bar{s}^2 + ()\bar{s}^4$ – reflect the symmetry $\bar{s} \leftrightarrow -\bar{s}$

• the equilibrium value of $\bar{s} = \bar{s}(T, b)$: from minimization of $\Psi_L(\bar{s})$ with respect to $\bar{s}$ (performed at fixed T and b)

• validity only near the critical point $(T \to T_C,\ b \to 0)$

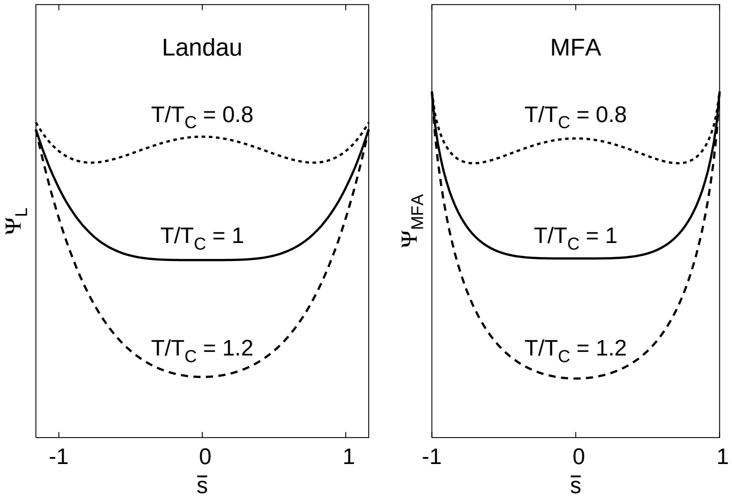
• the MFA provides a similar function (defined for $|\bar{s}| \leq 1$): a in $\Phi_1(a)$, Eq. (21), is replaced by $\bar{s} = \tanh(\beta a)$, Eq. (8), which yields [see also Eq. (22)]:

$$\Psi_{MFA}(\bar{s}) = -\frac{\mathcal{J}}{2}\bar{s}^2 - b\bar{s} + k_B T\left(\frac{1+\bar{s}}{2}\ln\frac{1+\bar{s}}{2} + \frac{1-\bar{s}}{2}\ln\frac{1-\bar{s}}{2}\right) \qquad (28)$$

• the functions $\Psi_L(\bar{s})$ and $\Psi_{MFA}(\bar{s})$ are very similar (for $|\bar{s}| \ll 1$); a comparison of their Taylor expansions (around $\bar{s} = 0$) yields $2c_2 = k_B$ and $12c_4 = k_B T_C = \mathcal{J}$ $\Longrightarrow$

- quantitative agreement between the MFA and the Landau theory in the critical region
- identical critical exponents (β, γ, δ) in both approaches

The functions $\Psi_L(\bar{s})$ and $\Psi_{MFA}(\bar{s})$
in absence of external magnetic field ($b = 0$)



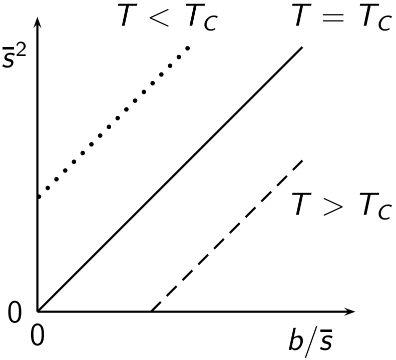
- the equilibrium value of $\bar{s}$ follows from Eq. (27),

$$\frac{\partial \Psi_L(\bar{s})}{\partial \bar{s}} = 0 \quad \Longrightarrow \quad b = 2c_2(T - T_C)\bar{s} + 4c_4\bar{s}^3 \,, \qquad (29)$$

which can be recast as

$$\frac{b}{\bar{s}} = 2c_2(T - T_C) + 4c_4\bar{s}^2$$

and depicted by means of the Arrott plot (isotherms – straight lines)



3.6 Critical behavior

• the condition for $\bar{s}$ in the Landau theory, Eq. (29), can also be rewritten with definition of $t \equiv |T - T_C|$ as

$$\left(bt^{-3/2}\right) = \pm 2c_2 \left(\bar{s}t^{-1/2}\right) + 4c_4 \left(\bar{s}t^{-1/2}\right)^3 , \qquad (30)$$

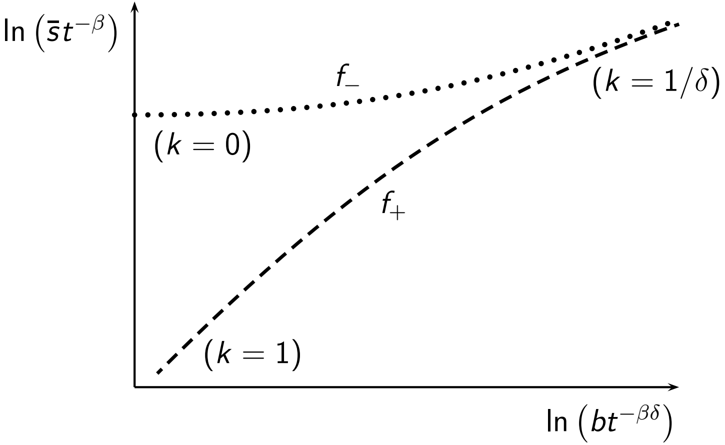
where the $+ \, (-)$ sign refers to $T > T_C$ $(T < T_C)$;

$\Longrightarrow$ $\bar{s}t^{-1/2}$ ('rescaled magnetization') depends only on $bt^{-3/2}$ ('rescaled field') and on the sign of $T - T_C$

• in experiment (and more sophisticated theories) and near the critical point, one finds similarly (β, δ – critical exponents)

$$\bar{s}t^{-\beta} = f_{\pm}\left(bt^{-\beta\delta}\right) , \qquad (31)$$

so that the full dependence $\bar{s} = \bar{s}(T, b)$ reduces to two functions $f_{\pm}$ of a single variable



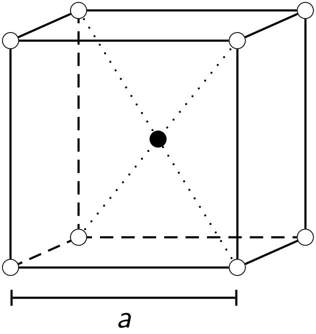
(k values – slopes of the asymptotic straight lines)

4 Complex magnetic orders

• simple structures can exhibit complex magnetic orders (at low temperatures) featured by a reciprocal-space vector $\mathbf{k}_0$ $\Longrightarrow$ a real-space structure with period $\Lambda = 2\pi/|\mathbf{k}_0|$ often *incommensurate* with the underlying lattice parameters

• examples on bcc lattice:

- Fe: ferromagnet, trivial $\mathbf{k}_0 = (0, 0, 0)$
- Cr: spin density wave, $\mathbf{k}_0 = (2\pi/a)(0.952, 0, 0)$
- Eu: spin spiral, $\mathbf{k}_0 = (2\pi/a)(0.27, 0, 0)$



• tendency to formation of non-ferromagnetic orders can be understood from the MFA conditions, Eq. (5),

$$\bar{s}_m = \tanh\left[\beta\left(b_m + \sum_n J_{mn}\bar{s}_n\right)\right] ,$$

applied to a simple (Bravais) lattice but without an assumption of equivalence of the quantities b_m and $\bar{s}_m$ for different lattice sites

• in the limit of high temperatures T and small applied fields b_m, these conditions reduce to a set of linear equations

$$\bar{s}_m = \beta b_m + \beta\sum_n J_{mn}\bar{s}_n , \tag{32}$$

where the spins $\bar{s}_m$ at all lattices sites are mutually coupled

• since $J_{mn} = J_{(m-n)0}$ due to the translational invariance of the Bravais lattice, Eq. (32) is of a convolution type $\Longrightarrow$ it can be solved using the lattice Fourier transformation:

$$\begin{aligned}
\tilde{s}(\mathbf{k}) &= \sum_m \exp(i\mathbf{k}\cdot\mathbf{T}_m)\,\bar{s}_m\,, \\
\tilde{b}(\mathbf{k}) &= \sum_m \exp(i\mathbf{k}\cdot\mathbf{T}_m)\,b_m\,, \\
\tilde{J}(\mathbf{k}) &= \sum_m \exp(i\mathbf{k}\cdot\mathbf{T}_m)\,J_{m0}\,, \qquad (33)
\end{aligned}$$

where $\mathbf{k}$ – a vector from the 1st Brillouin zone (BZ),
$\mathbf{T}_m$ – the m-th translational vector
(the vector of lattice site m)

- (a technical note)

- the standard Fourier transformation in 1D and its inverse are defined by

$$\tilde{f}(k) = \int_{-\infty}^{+\infty} \exp(\mathrm{i}kx)\, f(x)\, \mathrm{d}x\,,$$

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(-\mathrm{i}kx)\, \tilde{f}(k)\, \mathrm{d}k$$

- the convolution $h = f * g$ of two functions is defined by

$$h(x) = \int_{-\infty}^{+\infty} f(x-y)\, g(y)\, \mathrm{d}y$$

and it holds: $\tilde{h}(k) = \tilde{f}(k)\, \tilde{g}(k)$

• the original set of coupled relations, Eq. (32), is transformed into separate relations involving only a single $\mathbf{k}$ vector:

$$\begin{aligned} \tilde{s}(\mathbf{k}) &= \beta\tilde{b}(\mathbf{k}) + \beta\tilde{J}(\mathbf{k})\tilde{s}(\mathbf{k}) \qquad \Longrightarrow \\ \tilde{s}(\mathbf{k};T) &= \tilde{\chi}(\mathbf{k};T)\tilde{b}(\mathbf{k})\,, \quad \tilde{\chi}(\mathbf{k};T) = \frac{1}{k_B T - \tilde{J}(\mathbf{k})} \end{aligned} \tag{34}$$

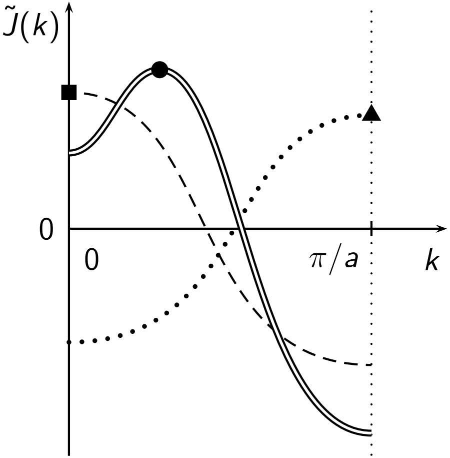
• the divergence of the solution $\tilde{s}(\mathbf{k};T)$, Eq. (34), leads to a critical temperature T_{cr} given in the MFA as

$$k_B T_{cr} = \max_{\mathbf{k}\in BZ} \tilde{J}(\mathbf{k}) \equiv \tilde{J}(\mathbf{k}_0)\,, \tag{35}$$

where $\mathbf{k}_0$ – the vector of the (complex) magnetic structure:

- ferromagnetism for $\mathbf{k}_0 = \mathbf{0}$ $\quad [\, \tilde{J}(\mathbf{0}) = \sum_m J_{m0} = \mathcal{J} \,]$
- $\mathbf{k}_0 \neq \mathbf{0}$ requires some pair interactions negative $(J_{mn} < 0)$

- example: 1-dimensional lattice with lattice parameter a, its 1st BZ is $-\pi/a \le k \le \pi/a$



■ $k_0 = 0$
ferromagnet

▲ $k_0 = \pi/a$
antiferromagnet
$\dots \uparrow\downarrow\uparrow\downarrow\uparrow \dots$

● $0 < k_0 < \pi/a$
complex order
$\Lambda = 2\pi/k_0$

5 Non-local susceptibility and spin-spin correlation functions

• in the paramagnetic state $(T > T_{cr})$, the linear relation between the small applied fields b_m and the resulting small values of $\bar{s}_m$ can be written quite generally as

$$\bar{s}_m(T) = \sum_n \chi_{mn}(T)\, b_n\,, \tag{36}$$

where the non-local susceptibilities $\chi_{mn}(T)$ are defined as

$$\chi_{mn}(T) = \left.\frac{\partial \bar{s}_m(T;\{b_j\})}{\partial b_n}\right|_0\,, \tag{37}$$

where the partial derivative is taken at all fields null, $b_j = 0$. The meaning of $\chi_{mn}(T)$ is obvious: it reflects the effect of a local field at site n on the average value of the spin at site m.

• for Bravais lattices, the susceptibilites $\chi_{mn}(T)$ are translationally invariant; their lattice Fourier transformation

$$\tilde{\chi}(\mathbf{k};T) = \sum_m \exp(i\mathbf{k}\cdot\mathbf{T}_m)\,\chi_{m0}(T)$$

is given in the MFA according to Eq. (34) by

$$\tilde{\chi}(\mathbf{k};T) = \left[k_B T - \tilde{J}(\mathbf{k})\right]^{-1} . \tag{38}$$

The values of $\chi_{mn}(T)$ can be obtained from the inverse lattice Fourier transformation

$$\chi_{m0}(T) = \frac{1}{\Omega_{BZ}} \int_{BZ} \exp(-i\mathbf{k}\cdot\mathbf{T}_m)\,\tilde{\chi}(\mathbf{k};T)\,\mathrm{d}^3\mathbf{k}\,, \tag{39}$$

where the integration is taken over the 1st BZ, the volume of which is Ω_{BZ}.

• the spin-spin correlation functions are defined as averages $\langle s_m s_n \rangle$ taken at temperature T ($T > T_{cr}$) and at all fields null, $b_j = 0$ $\quad (\implies \bar{s}_m = 0$ for all sites)

• in the MFA, the spin-spin correlation functions for different sites ($m \neq n$) reduce to zero, see Eq. (7)

• however, a general exact relation of the classical Boltzmann statistics (between the susceptibility and the correlation of fluctuations) allows one to express

$$\langle s_m s_n \rangle (T) \,=\, k_B T \, \chi_{mn}(T)\,, \tag{40}$$

which thus yields non-trivial correlation functions even in the MFA

• for a ferromagnet, the maximum value of $\tilde{\chi}(\mathbf{k};T)$ $\{=[k_B T - \tilde{J}(\mathbf{k})]^{-1}\}$ occurs at $\mathbf{k}=\mathbf{0}$ since

$$\tilde{J}(\mathbf{k}) = \mathcal{J} - Dk^2 \qquad \text{for} \quad k \equiv |\mathbf{k}| \to 0\,, \tag{41}$$

where $\mathcal{J} = \tilde{J}(\mathbf{0}) = k_B T_C$ and where the D $(D>0)$ is a spin-wave stiffness constant (for simplicity, we assume cubic lattices only). Consequently, the $\tilde{\chi}(\mathbf{k};T)$ reduces to

$$\tilde{\chi}(\mathbf{k};T) = \frac{D^{-1}}{\xi^{-2}(T)+k^2} \qquad \text{for} \quad k \to 0\,, \tag{42}$$

where the so-called correlation length $\xi(T)$ is defined by

$$\xi(T) = \sqrt{\frac{D}{k_B(T-T_C)}}\,. \tag{43}$$

• by extending the validity of Eq. (42)
$\{\ \tilde{\chi}(\mathbf{k};T) \sim [\xi^{-2}(T) + k^2]^{-1}\ \}$ to all values of $\mathbf{k}$
and by integrating over the whole reciprocal space in the inverse lattice Fourier transformation, Eq. (39),
we get the MFA spin-spin correlation functions as

$$\langle s_m s_n \rangle (T) \sim \frac{1}{d_{mn}} \exp\left[-\frac{d_{mn}}{\xi(T)} \right] , \tag{44}$$

where the $d_{mn} = |\mathbf{T}_m - \mathbf{T}_n|$ denotes the intersite distance. The relations described by Eq. (42) and Eq. (44) are called the Ornstein-Zernike behavior.

• the meaning of Eq. (44) is obvious: the spin-spin correlations are negligible for very distant sites $[d_{mn} > \xi(T)]$, but they are appreciable for nearby sites $[d_{mn} < \xi(T)]$

• the divergence of the correlation length for $T \to T_C^+$ given by Eq. (43) represents a special case of the critical behavior

$$\xi(T) \sim (T - T_C)^{-\nu} \tag{45}$$

with the MFA critical exponent $\nu = 1/2$, whereas more accurate theories yield values $\nu \approx 0.7$ (confirmed by experiments as well)

• this divergence is a characteristic feature of the phase transition; it corresponds to presence of big clusters [domains of size $\approx \xi(T)$] of spins pointing in the same direction

6 Properties of the MFA

• the MFA is qualitatively or semi-quantitatively correct in a number of cases; nevertheless, it exhibits several shortcomings:

- it yields a phase transition in any dimension
- for temperatures near the critical point: incorrect critical exponents
- for high temperatures: complete neglect of the magnetic short-range order $(\langle s_m s_n \rangle_{MFA} = 0)$
- for low temperatures: a too slow reduction of magnetization with increasing temperature, Eq. (16), whereas experiment gives the Bloch law: $\overline{s^z}(0) - \overline{s^z}(T) \sim T^{3/2}$

- the last shortcoming cannot be removed (within the MFA):

  ¶ the classical Heisenberg model yields:

$$\overline{s^z} = \mathcal{L}(\beta a)\,, \qquad a = b + \mathcal{J}\,\overline{s^z}\,,$$

  where $\mathcal{L}(x) = \coth(x) - x^{-1}$ – the Langevin function;
  $\Longrightarrow$ a very fast reduction: $\overline{s^z}(0) - \overline{s^z}(T) \sim T$

  ¶ the quantum Heisenberg model yields:

$$\overline{s^z} = \mathcal{B}_S(\beta a)\,, \qquad a = b + \mathcal{J}\,\overline{s^z}\,,$$

  where $\mathcal{B}_S(x)$ – the Brillouin function for the quantum atomic spin S (integer or half-integer);
  $\Longrightarrow$ a similar slow reduction as in Eq. (16)