

Physics 7240: Advanced Statistical Mechanics

Lecture 2: Magnetism: exact solutions and mean-field theories

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I. OUTLINE

- Background to magnetism
- Paramagnetism
- Spin exchange vs dipolar interaction
- Heisenberg model and crystalline anisotropies
- Ising model in low dimensions
- Mean-field and Landau theory of PM-FM transition

II. BACKGROUND

In this set of lectures we will study statistical mechanics of magnetic insulators. These are composed of local magnetic moments arising from atomic orbital charge currents and intrinsic electron and nuclear spin. For simplicity we will denote the combined angular momentum by dimensionless spin \mathbf{S} and the associated magnetic moment $\boldsymbol{\mu} = \mu\mathbf{S}$, where μ carries the units of magnetization with details that depend on the microscopics of the moment (spin, orbital, etc), that will not concern us here. The Hamiltonian of an isolated magnetic moment in the presence of a magnetic field is given by the Zeeman form,

$$H_Z = -\boldsymbol{\mu} \cdot \mathbf{B} = -\mu\mathbf{S} \cdot \mathbf{B}, \quad (1)$$

For quantum spins, as usual the micro-states are labeled by the total spin (with magnitude squared eigenvalue $S(S+1)$) and by a projection of \mathbf{S} (conveniently taken along \mathbf{B}), that takes on $2S+1$ values $s \in \{-S, -S+1, \dots, S-1, S\}$, with energy eigenvalues, $E_s = s\mu B$. For large S , the spectrum E_s is dense ($\Delta E_s \ll k_B T$) and the sum over s states reduces to an integral, that we expect to be equivalent to $\int d\Omega$. For $S\mu B \ll k_B T$ it ranges over the full 4π steradians of orientations of a classical spin, \mathbf{S} .

III. CURIE PARAMAGNETISM OF LOCAL MOMENTS IN AN INSULATOR

For the noninteracting spin Hamiltonian, (1) the thermodynamics, heat capacity, magnetic susceptibility as well as other response and correlation functions are straightforwardly

computed. The thermodynamics is contained in the partition function, that for a single spin is given by

$$Z_1(B) = e^{-\beta F} = \sum_{s=-S}^S e^{-s\mu B/k_B T} = \frac{\sinh[(2S+1)\mu B/(2k_B T)]}{\sinh[\mu B/(2k_B T)]}, \quad (2)$$

For N noninteracting spins $Z_N = Z_1^N$, the free energy $F_N = NF_1$, and the magnetization density is given by

$$m(B) = -n\partial F_1/\partial B = n\mu S B_S(S\mu B/k_B T), \quad (3)$$

where $B_S(x)$ is the Brillouin function, $B_S(x) = (1 + \frac{1}{2S}) \coth[(1 + \frac{1}{2S})x] - \frac{1}{2S} \coth(\frac{x}{2S}) \approx_{x \rightarrow 0} \frac{1}{3}(1 + 1/S)x$. For $S = 1/2$ (the so-called Ising case), the partition function and magnetization reduce to

$$Z(B) = [e^{\mu B/k_B T} + e^{-\mu B/k_B T}]^N = [2 \cosh(\mu B/k_B T)]^N, \quad (4)$$

$$m(B) = \frac{\mu N}{V Z(B)} [e^{\mu B/k_B T} - e^{-\mu B/k_B T}] = -\frac{\partial}{\partial B} F, \quad (5)$$

$$= n\mu \tanh(\mu B/k_B T). \quad (6)$$

It can be verified that above expressions display the correct quantum (low T) and classical (large T) limits. In the latter, classical limit $\mu B \ll k_B T$ the result reduces to Curie linear susceptibility (using $\coth x \approx 1/x + x/3 + \dots$)

$$\chi_C(B=0, T) = \frac{\partial m}{\partial B} \Big|_{B \rightarrow 0} = \frac{1}{3} n \mu^2 \frac{S(S+1)}{k_B T} \equiv \frac{C}{T}, \quad (7)$$

with C the Curie constant and $m \approx \chi(T)B$ exhibiting a linear response in this regime. This $1/T$ linear susceptibility behavior is a generic experimental signature of independent local moments, with the amplitude C a measure of the size of the magnetic moment and the associated spin. At finite T the susceptibility is finite and paramagnetic (i.e., magnetization is along the applied magnetic field and vanishes with a vanishing field), only diverging at a vanishing temperature. This captures the fact that in a classical regime, as $T \rightarrow 0$ a nonzero magnetization is induced in response to an infinitesimal field, as disordering thermal fluctuations vanish. For sufficiently low T a quantum regime of large Zeeman gaps $\mu B \gg k_B T$ is reached, and magnetization density saturates at its maximum value of $n\mu S$, and susceptibility and heat capacity vanish exponentially. In the opposite limit of high temperature and low field, $S\mu B \ll k_B T$, all states are equally accessible, entropy dominates and the free energy approaches $-k_B T \ln(2S+1)$. These limits are illustrated in Figs.(1) and (2). As we will see below, interactions between local moments lead to a far richer behavior.

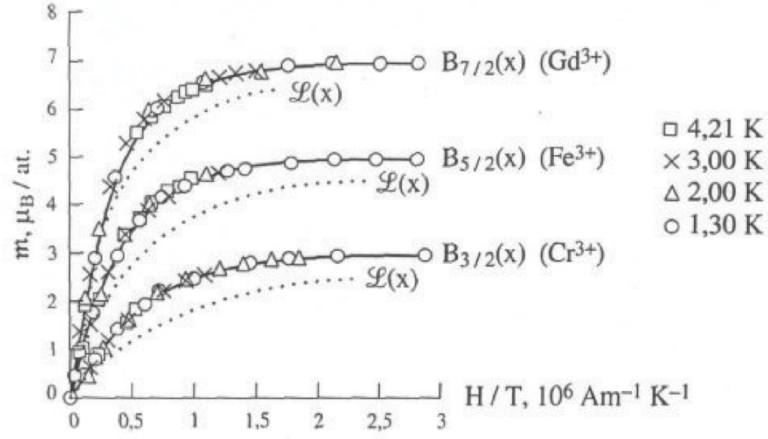


FIG. 1: Reduced magnetization curves for three paramagnetic salts and comparison with Brillouin theory prediction, from Ref.[20].

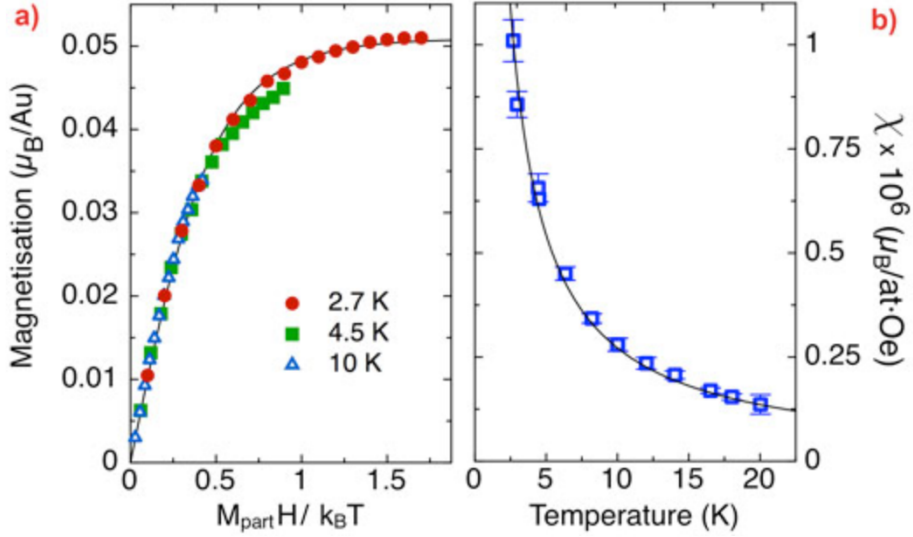


FIG. 2: Magnetization and corresponding Curie susceptibility in gold (Au) nanoparticles, measured at several temperatures up to $H = 17$ Tesla. Reduced magnetization curves for three paramagnetic salts and comparison with Brillouin theory prediction, from Ref.22.

IV. SPIN-SPIN EXCHANGE INTERACTION

As a general “More is Different” (P. W. Anderson) theme of condensed physics, its richness arises from interactions (gases are boring, but liquids are interesting). This of

course also extends to magnetism where the rich array of magnetic phases observed in solids is due to interaction between magnetic moments.

Now, based on magnetostatics one may naturally guess that interaction between spins is due to dipolar interaction between the associated magnetic moments

$$H_{dipole-dipole} = \frac{\mu_0}{4\pi r^3} [\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - 3(\boldsymbol{\mu}_1 \cdot \hat{\mathbf{r}})(\boldsymbol{\mu}_2 \cdot \hat{\mathbf{r}})], \quad (8)$$

where r is the distance between and $\hat{\mathbf{r}}$ is the unit vector connecting $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$. Using μ_B as the scale for the magnetic moment and Bohr radius r_0 as a measure of inter-moment spacing in a solid, an estimate of the dipole-dipole interaction energy is given by

$$E_{dipole-dipole} \approx \frac{\mu_0}{4\pi} \frac{\mu_B^2}{a_0^3} = \left(\frac{e^2}{4\pi\epsilon_0\hbar c} \right)^2 \frac{e^2}{16\pi\epsilon_0 a_0} \approx \left(\frac{1}{137} \right)^2 E_{Ry} \approx 5 \times 10^{-4} eV \approx \text{few Kelvin}, \quad (9)$$

and is just quite insignificant for ordering on the eV energy scale (10,000 Kelvin) relevant to magnetic solids, though can be important as a secondary scale for determining crystalline magnetic anisotropy.

Although at first sight quite paradoxical (since classically it is spin-independent), it is the much larger (order of eV) Coulomb interaction, together with quantum mechanics (via the Pauli principle that brings the spin configuration into the problem), that is responsible for magnetism in solids.

V. HEISENBERG MODEL

We leave the microscopic details of the spin exchange mechanism to a course on solid state physics. The result is that spins at sites \mathbf{R}_i and \mathbf{R}_j , interact via the so-called Heisenberg Hamiltonian

$$H_H = -\frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (10)$$

where J_{ij} is the corresponding exchange energy that can be positive (ferromagnetic) or negative (antiferromagnetic), tending to align or anti-align ij spins, respectively. In the quantum regime, this Hamiltonian is highly nontrivial (despite its deceptively simple quadratic form) as $\hat{\mathbf{S}}_i$ are operators, and thus H_H is supplemented by a nonlinear spin-commutation relation

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon_{\alpha\beta\gamma} S_i^\gamma, \quad (11)$$

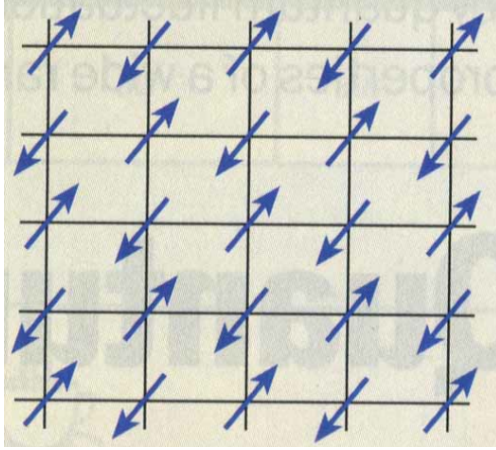


FIG. 3: Lattice of interacting spins (magnetic moments), exhibiting an antiferromagnetic (AFM) classical order (figure from Subir Sachdev).

leading to quantum spin fluctuations even at zero temperature.

Even in the classical limit, (10) can be highly nontrivial, with potentially competing exchange interactions, J_{ij} , exhibiting rich phenomenology. As we will see below, the key consequence of the exchange interaction is that (in contrast to noninteracting spins, that, as we saw above, do not order in the absence of a magnetic field) a lattice of spins can undergo a magnetic ordering phase transition below a critical temperature, T_c into a configuration that strongly depends on sign and strength of J_{ij} , lattice structure and dimensionality.

We note that this ideal Heisenberg Hamiltonian has a full $SU(2)$ spin-rotational invariance, with spin orientation independent of the orbital (e.g., bond) orientations \mathbf{R}_{ij} . As we discuss below, physical magnets exhibit important deviation from this idealization due to spin-orbit interaction, that results in the so-called crystal-symmetry and other $SU(2)$ symmetry-breaking fields.

In the presence of an external magnetic field \mathbf{B} , H_H must be supplemented by the Zeeman interaction, (1), that for strong fields can overwhelm the exchange, aligning all the moments along \mathbf{B} .

VI. MAGNETIC ANISOTROPIES

In real crystals, spin-orbit interaction breaks full global $SU(2)$ spin rotational invariance, introducing coupling of spin orientation with the crystalline axes. The form of these, so-

called, crystalline anisotropies strongly depends on the atomic element, size of the spin, symmetry of the lattice and order of the interaction. In a cubic lattice to quadratic order in spins, no anisotropies appear (with lowest order appearing at quartic order as S_α^4). In tetragonal crystals, the Heisenberg model becomes

$$H_{ani} = -\frac{1}{2} \sum_{i,j} J_{ij} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z). \quad (12)$$

For $\Delta > 1$ the ordering is along z axis (uniaxial axis of the tetragonal crystal), the so-called “easy axis” Ising anisotropy. In the extreme limit of low energies the model reduces to the Ising model

$$H_{Ising} = -\frac{1}{2} \sum_{i,j} J_{ij} S_i^z S_j^z. \quad (13)$$

Since only commuting S_i^z operators appear, in this Ising limit the model is classical (i.e., no quantum fluctuations) and at $T = 0$ clearly exhibits classical magnetic order determined by the form of the exchange couplings J_{ij} .

Quantum fluctuations re-emerge in the presence of a *transverse* (to easy Ising axis) field, described by the transverse-field Ising (TFI) Hamiltonian

$$H_{TFI} = -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x, \quad (14)$$

where in the simplest case the exchange J_{ij} can be taken to be local (nonzero only for nearest neighbors, vanishing otherwise) and uniform transverse field h . In above we specialized to a simplest case of spin-1/2, allowing us to express the Hamiltonian in terms of the Pauli matrices $\sigma^x, \sigma^y, \sigma^z$ (absorbing the factor $\mu/2$ into the parameters J, h). As we will see below, this 1d quantum model maps onto 2d classical model and is therefore exactly solvable, exhibiting a quantum (at $T = 0$) FM-PM transition as a function of h/J . Amazingly, via Jordan-Wigner transformation it also maps onto a one-dimensional p-wave superconductor, which is the easiest way to solve the 2d classical and the TF Ising models.

In the opposite case of $|\Delta| < 1$, the spins order in the isotropic transverse to the uniaxial axis, in which (to quadratic order in spins) the so-called “easy plane” ordering is isotropic. In the extreme case the model reduces to the so-called XY model,

$$H_{XY} = -\frac{1}{2} \sum_{i,j} J_{ij} (S_i^x S_j^x + S_i^y S_j^y) = -\frac{1}{2} \sum_{i,j} J_{ij} \mathbf{S}_i^\perp \cdot \mathbf{S}_j^\perp. \quad (15)$$

In addition, for $S > 1/2$, a single-ion anisotropy $H_{ion} = -D \sum_i (S_i^z)^2$ can also appear in tetragonal crystals. Because S_i^z does not commute with \mathbf{S}_i^\perp , such anisotropy D can drive a quantum phase transition out of the XY-ordered ground state.

It is convenient to choose the quantization axis along the tetragonal uniaxial axis z and rewrite the Hamiltonian in terms of spin raising and lowering operators

$$S_i^+ = S_i^x + iS_i^y, \quad S_i^- = S_i^x - iS_i^y,$$

which reduces the Hamiltonian to

$$H = -\frac{1}{2} \sum_{i,j} J_{ij} \left(\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + \Delta S_i^z S_j^z \right). \quad (16)$$

This form reminds us of the quantum nature of the Heisenberg and XY (but not Ising) models. It also emphasizes its relation to the bosonic hopping problem, where spin exchange corresponds to a destruction of S_z quanta at site j and its creation at site i , and visa versa. As we will see, beyond a planar ferromagnet, XY model has a large number of diverse physical realizations, such as charge density waves, superfluids, spin-density wave, etc. For example, the two-component real spin, $\mathbf{S} = (S_x, S_y)$ naturally maps onto a single complex superfluid order parameter $\Psi = S_x + iS_y$.

VII. ISING MODEL

As we learned in the previous section, starting with an SU(2) invariant Heisenberg model and adding Ising crystalline anisotropies, reduces it to an Ising model with commuting S_z -only spin components. Quantum fluctuations re-emerge in the presence of a *transverse* (to easy Ising axis) field, described by the transverse-field Ising model (TFIM) Hamiltonian

$$H_{TFI} = -\frac{1}{2} \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z - \sum_i (h_x \sigma_i^x + h \sigma_i^z), \quad (17)$$

where we have also added a longitudinal external field h .

In general (spatial) dimensions $d > 2$ this model is not solvable, even in the classical limit, but it is in the quantum case of 1+1d (space+time dimensions) and also in the 1+0d and 2+0d classical case of $h_x = 0$, with the latter intimately related to the former, as we will see below.

A. Classical 1d Ising model

Let us first focus on the simplest case of a classical 1d model in a homogenous external longitudinal field with nearest neighbors exchange interactions (dropping superscript “z”),

$$H_{1d} = - \sum_{i=1}^N [J\sigma_i\sigma_{i+1} + h\sigma_i], \quad (18)$$

with periodic boundary conditions (i.e., closed spin-1/2 chain on a ring), with N spins and $\sigma_{N+1} = \sigma_1$, and thus last exchange term is $-J\sigma_N\sigma_1$. The corresponding partition function is given by,

$$\begin{aligned} Z &= \sum_{\{\sigma_i\}} e^{\sum_{i=1}^N [J\sigma_i\sigma_{i+1} + h\sigma_i]}, \\ &= \sum_{\{\sigma_i\}} T_{\sigma_1\sigma_2} T_{\sigma_2\sigma_3} \dots T_{\sigma_N\sigma_1} \equiv \text{Trace}[\hat{T}^N], \\ &= \lambda_+^N + \lambda_-^N, \end{aligned} \quad (19)$$

where I chose to measure energies J, h in units of thermal energy $k_B T$, $\sum_{\{\sigma_i\}} \equiv \sum_{\sigma_1=\pm 1} \sum_{\sigma_2=\pm 1} \dots \sum_{\sigma_N=\pm 1}$ corresponds to N independent sums over N spins, and λ_{\pm} are two eigenvalues of \hat{T} . The last expression for Z expressed it in terms of a trace of a N th power of a “transfer matrix” \hat{T} read off by inspection to be given by

$$T_{\sigma,\sigma'} = e^{J\sigma\sigma' + \frac{1}{2}h(\sigma+\sigma')} = \begin{pmatrix} T_{1,1} & T_{1,-1} \\ T_{-1,1} & T_{-1,-1} \end{pmatrix} = \begin{pmatrix} e^{J+h} & e^{-J} \\ e^{-J} & e^{J-h} \end{pmatrix}, \quad (20)$$

$$\begin{aligned} &= (e^J \cosh h) 1 + (e^J \sinh h) \sigma^z + e^{-J} \sigma^x \equiv (e^J \cosh h) 1 + \vec{b} \cdot \vec{\sigma}, \\ &= a [(\cosh g) 1 - \hat{n} \cdot \vec{\sigma} (\sinh g)] \equiv a e^{-g\hat{n} \cdot \vec{\sigma}}, \end{aligned} \quad (21)$$

where in above equality we expressed \hat{T} in terms of Pauli matrices and the identity matrix 1, defined a pseudo-magnetic field $\vec{b} = (e^{-J}, 0, e^J \sinh h)$ (by analogy with quantum single spin Hamiltonian in a field) and in the last equality used their properties to express \hat{T} as an exponential of a linear combination of Pauli matrices, with $a^2 = e^{2J} \cosh^2 h - |\vec{b}|^2 = e^{2J} \cosh^2 h - e^{2J} \sinh^2 h - e^{-2J}$.

1. zero field $h = 0$

For $h = 0$ the eigenvalues λ_{\pm} are easily evaluated, since eigenvalues of σ^x are ± 1 , giving $\lambda_+ = 2 \cosh J$ and $\lambda_- = 2 \sinh J$, which gives,

$$Z(h = 0) = (2 \cosh J)^N + (2 \sinh J)^N \approx (2 \cosh J)^N, \quad (22)$$

where largest eigenvalue λ_+ dominates in the thermodynamic limit, giving $F(h = 0) \approx N \ln(2 \cosh J)$.

I note that above result can be immediately obtained by using bond variables $\tau_i = \sigma_i \sigma_{i+1}$ as the basic degree of freedom. This is possible for open boundary conditions, where τ_i contains same information as σ_i , up to a factor of 2 due to the one end spin. The resulting partition function is then simply

$$Z = 2 \sum_{\{\tau_i = -1, 1\}} e^{-J \sum_{i=1}^{N-1} \tau_i} = 2(2 \cosh J)^{N-1},$$

which in the $N \gg 1$ limit matches the exact one above computed terms of σ_i .

For periodic boundary conditions, there are as many bond variables as spins (N) except that there are two spin configurations for every set of bond configurations. However, there is also an obvious but important constraint, $\prod_i^N \tau_i = 1$. This constraint must be faithfully implemented. To this end we introduce $C = \frac{1}{2} \sum_i^N (1 - \tau_i)$, that counts the total number of negative τ_i bonds. We can use C to project out the *odd* number of negative τ_i 's configurations (that don't satisfy $\prod_i^N \tau_i = 1$) out of the partition function using projector $P = \frac{1}{2}(1 + e^{i\pi C})$ (which is 0 (1) if C is odd (even)). Imposing this constraint on Z expressed in terms of τ_i s we recover the exact result Eq. (22), above.

Calculating the free energy $F = -k_B T \ln Z \approx -N k_B T \ln[2 \cosh(J/k_B T)]$ and computing the average energy $E(T)$ and heat capacity $C_V(T)$ we find

$$E(T) = -\partial \ln Z / \partial \beta \approx -N J \tanh(J/k_B T), \quad (23)$$

$$C_V(T) = \partial E / \partial T \approx k_B N (J/k_B T)^2 / \cosh^2(J/k_B T), \quad (24)$$

where the approximate result was computed in the thermodynamic limit, $N \gg 1$, dominated by the largest eigenvalue λ_+ . These have sensible behavior: as expected $E(T)$ vanishes in high T limit (no correlations between spins) and saturating at $-JN$ in the low $T \ll J/k_B$ limit, and $C_V(T)$ displays the standard Schottky peak form (decaying exponentially, $e^{-2J/k_B T}$

at low T and as $1/T^2$ at high T). The key observation is that these functions are analytic in T and thus display no sign of a phase transition in a 1d Ising model, as expected from our numerous further discussions.

We can also use transfer matrix methods to compute spin correlation functions, e.g.,

$$\begin{aligned}\langle \sigma_k \rangle &= \frac{1}{Z} \sum_{\{\sigma_i = \pm 1\}} e^{J \sum_{i=1}^N \sigma_i \sigma_{i+1}} \sigma_k = \frac{1}{Z} \text{Tr} [T^{N-k+1} \tau_3 T^{k-1}], \\ &\approx \frac{1}{\lambda_+^N} \sum_{\sigma = \pm} \langle \sigma | T^{N-k+1} | \sigma \rangle \langle \sigma | \tau_3 | \sigma \rangle \langle \sigma | T^{k-1} | \sigma \rangle = \sum_{\sigma = \pm} \langle \sigma | \tau_3 | \sigma \rangle = 0,\end{aligned}\quad (25)$$

$$\begin{aligned}\langle \sigma_l \sigma_k \rangle &= \frac{1}{Z} \sum_{\{\sigma_i = \pm 1\}} e^{J \sum_{i=1}^N \sigma_i \sigma_{i+1}} \sigma_l \sigma_k = \frac{1}{Z} \text{Tr} [T^{N-l+1} \tau_3 T^{l-k} \tau_3 T^{k-1}], \\ &\approx \frac{1}{\lambda_+^N} \sum_{\sigma, \sigma' = \pm} \langle \sigma | T^{N-l+1} | \sigma \rangle \langle \sigma | \tau_3 | \sigma' \rangle \langle \sigma' | T^{l-k} | \sigma' \rangle \langle \sigma' | \tau_3 | \sigma \rangle \langle \sigma | T^{k-1} | \sigma \rangle, \\ &\approx \sum_{\sigma' = \pm} \left(\frac{\lambda_{\sigma'}}{\lambda_+} \right)^{l-k} |\langle + | \tau_3 | \sigma' \rangle|^2 = |\langle + | \tau_3 | + \rangle|^2 + |\langle + | \tau_3 | - \rangle|^2 \left(\frac{\lambda_-}{\lambda_+} \right)^{l-k}, \\ &\approx e^{-|l-k|/\xi(T)},\end{aligned}\quad (26)$$

where τ_3 is the 3rd Pauli matrix, and we used eigenstates of \hat{T} (which are $|\pm\rangle = 2^{-1/2}(1, \pm 1)$) decomposition (analogue of Lehmann spectral decomposition) to find that magnetization vanishes and the correlation function decays exponentially with correlation length,

$$\xi(T) = \frac{1}{\ln(\lambda_+/\lambda_-)} = -1/\ln[\tanh(J/k_B T)] \approx_{k_B T \ll J} \frac{1}{2} e^{2J/k_B T}. \quad (27)$$

The correlation length is finite and analytic at all temperatures and at low T diverges exponentially, corresponding to the separation between decorrelating domain-walls of energy $2J$. This is all consistent with the absence of phase transition in the classical, 1 + 0d Ising model.

2. finite longitudinal field $h \neq 0$

The eigenvalues of \hat{T} in the presence of an external longitudinal field h are also easily found (particularly utilizing connection to quantum single spin Hamiltonian in a field \vec{b} , where $E_{\pm} = \pm|\vec{b}|$), and are given by,

$$\lambda_+ = e^J \cosh(h) + \sqrt{e^{2J} \sinh^2 h + e^{-2J}}, \quad (28)$$

$$\lambda_- = e^J \cosh(h) - \sqrt{e^{2J} \sinh^2 h + e^{-2J}}, \quad (29)$$

from which the free energy $F \approx -k_B T N \ln(\lambda_+)$ and all other thermodynamic quantities, e.g., the magnetization $\langle \sigma \rangle = -\partial F / \partial h$ can be computed. Simple analysis shows that for $h = 0$ indeed the magnetization vanishes at all temperatures, as in a simple paramagnet. This is consistent with the earlier findings and in particular the absence of the continuous phase transition and the absence of the magnetized phase in the 1d Ising model at zero field.

3. 1+0d classical Ising \rightarrow 0+1d quantum spin in a field

We finally note can be put into an exponential form $\hat{T} = a e^{-\tau \hat{H}_Q}$, in terms of a constant a , arbitrary constant τ (with condition that $N\tau = \beta$), and a 2×2 matrix $\hat{H}_Q = g \hat{n} \cdot \vec{\sigma}$, using properties of Pauli matrices that $e^{-g \hat{n} \cdot \vec{\sigma}} = (\cosh g) 1 - \hat{n} \cdot \vec{\sigma} (\sinh g)$. The latter can be interpreted as an equivalent quantum Hamiltonian of the 0+1 dimensional i.e., a single quantum spin problem in a magnetic field. For $h = 0$, the transfer matrix

$$\hat{T} = e^J 1 + e^{-J} \sigma^x,$$

is particularly simple, for which we find $\tau H_Q = g \sigma^x$, with

$$\begin{aligned} g &= -\frac{1}{2} \ln(\tanh J) \leftrightarrow \tanh g = -e^{-2J}, \\ a &= \sqrt{2 \sinh 2J}. \end{aligned} \tag{30}$$

The corresponding quantum partition function is

$$Z = \text{Trace} \left[e^{-\beta_Q \hat{H}_Q} \right],$$

where up to a constant $\hat{H}_Q = -h_x \sigma^x$, with $h_x = g$, $\beta_Q = N$. The latter relation dictates that the quantum spin is at an effective quantum temperature that vanishes in the thermodynamic limit $N \rightarrow \infty$. The correlation length in this quantum approach is proportional to the inverse of the excitation gap, which is set by g , giving $\xi \sim 1/g$, in agreement with classical prediction, above, Eq. (27).

Thus we indeed find an amazing result that (as we will see later in the course is quite general extending beyond Ising model) thermodynamics of the 1d classical Ising chain is equivalent to that of a 0+1d single quantum spin a magnetic field and temperature that vanishes in a thermodynamic limit.

B. Classical 2d Ising model and quantum 1d Ising model in a transverse field

Transfer matrix treatment can also be used to solve an anisotropic 2d classical Ising model, with sites labelled by $(x, y) \equiv (i, \tau)$, with N_v, N_h rows and columns and anisotropic exchanges,

$$H_{2dIsing} = - \sum_{i, \tau=1}^{N_h, N_v} [J_h \sigma_i^\tau \sigma_{i+1}^\tau + J_v \sigma_i^\tau \sigma_i^{\tau+1}]. \quad (31)$$

This model can be turned into a 1+1d quantum Ising model in the presence of a transverse magnetic field,

$$\hat{H}_{TFI} = - \sum_{i=1}^{N_h} [J_h \hat{\sigma}_i^3 \hat{\sigma}_{i+1}^3 + h_\perp \hat{\sigma}_i^1]. \quad (32)$$

The latter quantum model can be solved using Jordan-Wigner fermion representations of the spin operators, $\vec{S} = \frac{1}{2} \vec{\sigma}$,

$$S_i^+ = c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j}, \quad S_i^- = e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i, \quad S_i^z = c_i^\dagger c_i - \frac{1}{2}. \quad (33)$$

where c_i, c_i^\dagger satisfy usual fermion anticommutation algebra

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = 0, \quad \{c_i^\dagger, c_j^\dagger\} = 0.$$

This representation allows one to map the TFIM onto free, spinless fermions Hamiltonian when expressed in terms of c_i, c_i^\dagger .

Spin raising and lowering operators are associated with fermion creation and annihilation operators and z-component of spin is associated with fermion site filling value (shifted by 1/2). This “naive” representation must be supplemented with the so-called “string operator” (the exponential multiplying c, c^\dagger above to ensure the correct spin-commutation (rather than fermion anticommutation) algebra on different sites.

By carefully taking into account the Jordan-Wigner “string” we can demonstrate that the string ensures that indeed above spin representation satisfies spin-1/2 algebra on the same site, and with spins simply commuting on distinct sites.

To see this, first note that on the same site i , strings involves fermion number operator on site distinct from the fermion operator and thus commutes with the fermion operators. Thus,

$$[S_i^+, S_i^-] = c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j} e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i - e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j}, \quad (34)$$

$$= c_i^\dagger c_i - c_i c_i^\dagger = 2(n_i - 1/2) = 2S_z. \quad (35)$$

as required for spin algebra. On distinct sites, $i < j$, there is a nontrivial commutation relation between the two strings and between a string and a fermion operator. To flush this out we first note that on the Hilbert space $|0\rangle, |1\rangle$ a piece of the string at i , $e^{-i\pi c_i^\dagger c_i} = 1 - 2c_i^\dagger c_i$, giving ± 1 for $n_i = 0, 1$, respectively. Thus, $[e^{-i\pi c_i^\dagger c_i}, c_i^\dagger] = e^{-i\pi c_i^\dagger c_i} c_i^\dagger - c_i^\dagger e^{-i\pi c_i^\dagger c_i} = (1 - 2c_i^\dagger c_i)c_i^\dagger - c_i^\dagger(1 - 2c_i^\dagger c_i) = -2c_i^\dagger = -2c_i^\dagger(1 - 2c_i^\dagger c_i) = -2c_i^\dagger e^{-i\pi c_i^\dagger c_i}$, i.e.,

$$e^{-i\pi c_i^\dagger c_i} c_i^\dagger = -c_i^\dagger e^{-i\pi c_i^\dagger c_i} \rightarrow \{e^{-i\pi c_i^\dagger c_i}, c_i^\dagger\} = 0$$

. Armed with this we find

$$[S_i^+, S_j^-] = c_i^\dagger e^{i\pi \sum_{k<i} c_k^\dagger c_k} e^{-i\pi \sum_{l<j} c_l^\dagger c_l} c_j - e^{-i\pi \sum_{l<j} c_l^\dagger c_l} c_j c_i^\dagger e^{i\pi \sum_{k<i} c_k^\dagger c_k}, \quad (36)$$

$$= c_i^\dagger c_j e^{i\pi \sum_{k<i} c_k^\dagger c_k} e^{-i\pi \sum_{l<j} c_l^\dagger c_l} + c_j c_i^\dagger e^{-i\pi \sum_{l<j} c_l^\dagger c_l} e^{i\pi \sum_{k<i} c_k^\dagger c_k} = 0, \quad (37)$$

as required on different sites.

Using JW representation and carefully taking care of the string (as for above commutation relation) we can express the TFIM in terms of the JW fermions, finding

$$H_{TFIM} = -\frac{1}{4}J_h \sum_i (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}) - \frac{1}{2}h_\perp \sum_i (c_i^\dagger c_i - c_i c_i^\dagger),$$

with a crucial minus sign in the first term coming from the anticommutation relation between JW string and a fermion. Namely, the TFIM reduces to a quadratic fermionic Bogoluibov-like Hamiltonian.

It can then be straightforwardly diagonalized, such that in terms of true quasi-particles $\gamma_{\mathbf{k}}$, the Hamiltonian is

$$H_{TFIM} = \sum_{\mathbf{k}} E_{\mathbf{k}} \gamma_{\mathbf{k}}^\dagger \gamma_{\mathbf{k}} + E_0,$$

with the spectrum of excitations, $E_{\mathbf{k}}$, the gap (minimum excitation energy, related to the inverse of the Ising model's correlation length), and the ground state energy E_0 straightforwardly found, which gives the free energy and therefore all of thermodynamics of the classical 2d Ising model.

VIII. MEAN-FIELD THEORY OF FERROMAGNETISM IN CRYSTALLINE INSULATORS

Along with the phenomenological richness of interacting systems, comes the challenge of their solution. Except for one-dimension (where it can be solved by Bethe Ansatz) the

full quantum-mechanical Heisenberg model cannot be solved exactly. As we can see even the classical Ising model can only be solved in 1d or 2d. We thus embark on a variety of approximate analyses of this and other models, predicting appearance of magnetic orders and phase transitions between them. We defer a discussion of available exact solutions to other lectures.

The simplest and oldest approximate treatment of interacting systems in general is the so-called mean-field theory (MFT) approximation. The general idea is to replace the many-particle system by an effective one-particle Hamiltonian in the presence of an effective external field produced collectively by the remaining particles. The approximation is valid away from the transition, deep in the classically well-ordered and classically disordered states, where fluctuations are small. As we will see in the next lecture, MFT will break down near a critical point of a continuous phase transition, requiring a more sophisticated analysis, such as e.g., renormalization group theory, large-N approximation, etc.

A. Weiss mean-field theory

In the context of magnetic systems, MFT is known as Weiss mean-field theory (1907), where one replaces interacting spin model by a single spin in presence of an effective, self-consistently determined Weiss magnetic field.

To implement Weiss mean-field approximation on the classical Heisenberg model, we assume long-range magnetic order, characterized by a magnetization proportional to $\langle \mathbf{S}_i \rangle$, with spin then given by

$$\mathbf{S}_i = \langle \mathbf{S}_i \rangle + (\mathbf{S}_i - \langle \mathbf{S}_i \rangle),$$

a sum of the mean-field value and (presumed) small classical fluctuations. Inserting this into the Heisenberg Hamiltonian in the presence of an external field and neglecting the small fluctuations terms beyond first order, we obtain

$$H_{\text{mft}} = \frac{1}{2} \sum_{i,j} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \sum_{i,j} J_{ij} \langle \mathbf{S}_j \rangle \cdot \mathbf{S}_i - \mu \mathbf{B} \cdot \sum_i \mathbf{S}_i, \quad (38)$$

$$= \frac{1}{2} \sum_{i,j} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - \mu \mathbf{B}_{\text{eff}} \cdot \sum_i \mathbf{S}_i, \quad (39)$$

where the effective Weiss field is

$$\mathbf{B}_{\text{eff}} = \mathbf{B} + \frac{1}{\mu} \sum_j J_{ij} \langle \mathbf{S}_j \rangle,$$

that quite clearly gives a self-consistent mechanism to induce magnetic order, $\langle \mathbf{S}_j \rangle \neq 0$ even for a vanishing external magnetic field. The Weiss field on spin \mathbf{S}_i is generated by the neighboring spins. Since the above mean-field Hamiltonian, (39) is for a single spin, it can be solved exactly utilizing our earlier analysis, but now including an implicit self-consistency condition through \mathbf{B}_{eff} .

Focussing on the ferromagnetic state, we take $\langle \mathbf{S}_i \rangle \equiv \mathbf{S}_0 = \mathbf{m}/\mu$ to be spatially uniform, which allows us to directly utilize our analysis from Sec.III for Hamiltonian (39). From Eq.(3) we immediately find magnetization density along the applied field

$$m = n\mu S B_S [S\mu B_{\text{eff}}(m)/k_B T], \quad (40)$$

$$= n\mu S B_S [S\mu (B + \lambda m)/k_B T], \quad (41)$$

which gives a self-consistent equation for $m(B)$, with a constant $\lambda = J_0/(n\mu^2)$ and $J_0 \equiv \sum_j J_{ij}$ ($\approx Jz$ for nearest neighbors exchange model with z the lattice coordination number). We note that the magnetization, $m(B)$ is nonzero for any finite B , with spins biased to point along the external magnetic field. The above implicit equation can be solved graphically (or numerically), which for $B = 0$ is illustrated in Fig.4.

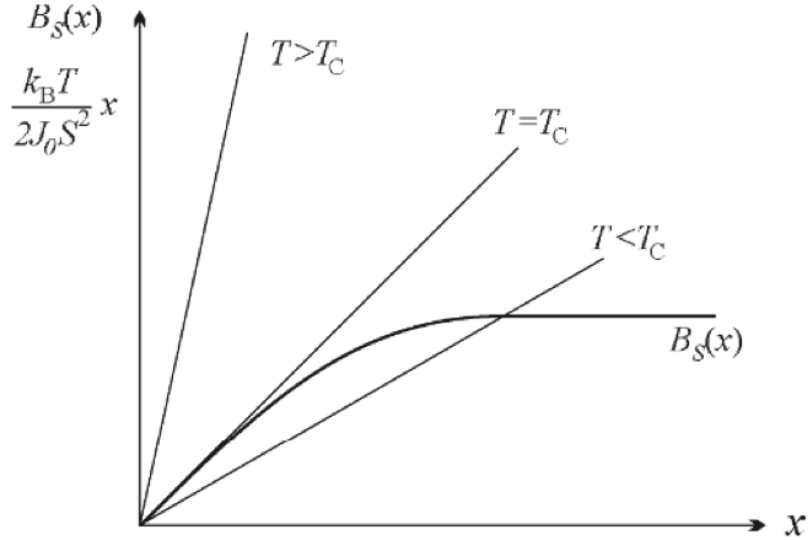


FIG. 4: Graphical determination of the mean-field magnetization $m(B = 0, T)$ from the intersection points of the Brillouin function $B_S(x)$ and straight lines of temperature-dependent slope (figure from Solyom, Solids State Physics I).

From its structure and

$$B_S(x) \approx_{x \rightarrow 0} \frac{1}{3}(1 + 1/S)x - \frac{1}{90S^3}(2S^3 + 4S^2 + 3S + 1)x^3, \quad (42)$$

$$\equiv \frac{1}{n\mu S} [(1 - a)m - bm^3], \quad (43)$$

$$(44)$$

it is clear that for sufficiently high $T > T_c$ (small prefactor in the argument of B_S), $a > 0$ and zero external field $B = 0$, there is only a single trivial paramagnetic solution $m = 0$ (Fig. 6). However, for $T < T_c$, $a < 0$ and there is also a nontrivial, ferromagnetic $m \neq 0$ solution, that can be shown to minimize the free energy for $T < T_c$. The critical Curie temperature T_c is easily found as the temperature at which the FM solution first appears and is given by

$$k_B T_c = \frac{1}{3} n \mu^2 S(S+1) \lambda, \quad (45)$$

$$= \frac{J_0}{3} S(S+1) = \frac{1}{3} J_0 \langle \mathbf{S}^2 \rangle, \quad (46)$$

quite naturally determined by the exchange constant J and a square of the spin operator with larger spin S (more classical) ordering at higher temperature.

This analysis is particularly simple for $S = 1/2$, in which case Weiss mean-field self-consistent equation is given by,

$$m = n\mu \tanh [\mu(B + \lambda m)/k_B T], \quad (47)$$

which for $B = 0$ has a simple Taylor expansion, rearranged in a suggestive way,

$$0 \approx -m + J_0/k_B T m - bm^3 = -\frac{\partial}{\partial m} F_{mft}[m]. \quad (48)$$

More generally, without Taylor expansion, utilizing the identity $\tanh(x) = d/dx [\ln \cosh(x)]$, Eq.(??) can be rewritten as a minimization of the mean-field free energy, given by

$$F_{mft}[m] = \frac{1}{2} \frac{1}{2} m^2 - \frac{n k_B T}{\lambda} \ln \cosh \left[\frac{\mu \lambda m}{k_B T} \right], \quad (49)$$

$$\approx \frac{1}{2} (1 - J_0/k_B T) m^2 + \frac{1}{4} m^4, \quad (50)$$

which has the famous Landau's " ϕ^4 " form, that we will encounter in the next sections.

Repeating this expansion for small B , we find the so-called Curie-Weiss linear linear response

$$m = \chi_{CW} B,$$

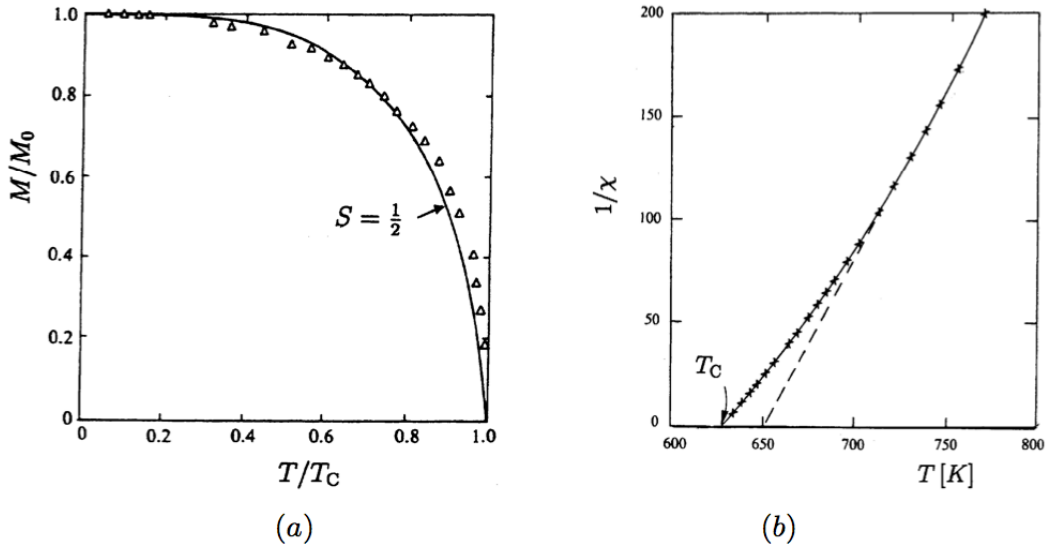


FIG. 5: Comparison of the measured magnetic properties of nickel [P. Weiss and R. Forrer, Ann. de Phys. 5, 153 (1926)] with the results obtained in the mean-field theory for $S = 1/2$. (a) Magnetization and (b) inverse susceptibility, as functions of temperature (figure from Solyom, Solids State Physics I).

with the susceptibility

$$\chi_{CW} = \frac{\chi_C}{|1 - T_c/T|} \sim |T - T_c|^{-\gamma},$$

that (in contrast to the paramagnetic Curie susceptibility χ_C) diverges at $T_c > 0$, where the system exhibits the paramagnetic-ferromagnetic continuous transitions. Above defines the susceptibility exponent γ , characterizing the degree of critical divergence at T_c , that in MFT is given by $\gamma = 1$. From above solution, for $B = 0$ we also find, that, while in the PM state $m = 0$, in the FM phase the magnetization grows as (see Fig.(5))

$$m \propto (T_c - T)^{1/2}, \quad \text{for } T < T_c,$$

and

$$m \propto B^{1/3}, \quad \text{at } T = T_c.$$

Similar mean-field analysis can be carried out for other magnetic states, for example the AFM Néel or spin-density wave states.

B. Fully-connected model: $d \rightarrow \infty$

An alternative but equivalent approach to Weiss mean-field theory is to instead consider a modified fully-connected Heisenberg model (sometimes referred to as infinite dimensional) with $J_{ij} = J/N$,

$$H_{\text{mft}}^{\infty} = -\frac{J}{2N} \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j - \mu \mathbf{B} \cdot \sum_i \mathbf{S}_i, \quad (51)$$

$$= -\sum_i \left[\frac{1}{2} J \mathbf{m} + \mu \mathbf{B} \right] \cdot \mathbf{S}_i, \quad (52)$$

$$= -N \left[\frac{1}{2} J \mathbf{m}^2 + \mathbf{B} \cdot \mathbf{m} \right], \quad (53)$$

where $\mathbf{m} = \frac{1}{N} \sum_j \mathbf{S}_j$ is the average magnetization, which therefore does not fluctuate, but needs to be determined self-consistently. Note that the rescaling $J \rightarrow J/N$ ensures that this fully-connected model has a well-defined thermodynamic $N \rightarrow \infty$ limit. Naturally, since all spins interact, the energy would otherwise go as JN^2 . Thus we scale down J by a factor of N (each exchange is vanishingly small) so as to get well-defined thermodynamic limit. Thus, the fully connected Heisenberg model is exactly solvable, as it corresponds to an effective single-spin problem in an internal magnetic field of constant magnetization \mathbf{m} due to all the remaining spins. Executing the same steps as for the Weiss MFT, above, we obtain the very same self-consistent equation for m , exhibiting a PM-FM phase transition.

I note that above two approaches are quite common alternatives in physics: find an approximate solution to an otherwise unsolvable model, or find an exact solution to a modified problem that is engineered to be exactly solvable.

We complement this canonical analysis by a microcanonical computation of the free energy for the Ising case. To this end we first note that for the fully-connected model, the energy as a function of m is exactly given by (53). The partition function and the associated Gibbs free energy can be computed in two steps,

$$Z(h, T) = e^{-\beta G(h, T)} = \sum_{\{\sigma_i\}} e^{-\beta H[\{\sigma_i\}, h]}, \quad (54)$$

$$= \sum_m e^{-\beta F(m, h, T)} = \sum_m \Omega(m) e^{-\beta E(m, h)} \quad (55)$$

by first summing over all $\Omega(m) = e^{S_E(m)/k_B}$ microstates $\{\sigma_i\}$ for fixed magnetization m , which gives Helmholtz free energy, $F(m, h, T) = E(m, h) - TS(m)$ (that we note is analytic

but not convex as function of m for $T < T_c$; see Fig.6), and then summing over m to obtain $G(h, T)$. This is possible for this model because the internal energy (53) is a function of m only and the entropy can be computed exactly for the Ising spin-1/2 model through multiplicity

$$\Omega(M) = \frac{N!}{[(N+M)/2]![(N-M)/2]!}, \quad (56)$$

a binomial coefficient counting the number of spin up/down configurations with a fixed M and N . Utilizing Sterling formula, $N! \approx (N/e)^N$ with $m = M/N \ll 1$ gives

$$\begin{aligned} S(m)/k_B &= \ln \Omega(m) = \ln \left[\frac{2^N}{(1+m)^{N(1+m)}(1-m)^{N(1-m)}} \right], \\ &= N \left[\ln 2 - \frac{1}{2}(1+m) \ln(1+m) - \frac{1}{2}(1-m) \ln(1-m) \right] \approx N \left[\ln 2 - \frac{1}{2}m^2 - \frac{1}{12}m^4 + \dots \right], \end{aligned} \quad (57)$$

consistent with the expectation that the entropy is maximum ($Nk_B \ln 2$, corresponding to random string of up/down spins) at $m = 0$, and precipitously quadratically decreasing with increasing magnetization m . Summing over m within the saddle-point approximation, namely by minimization of the exponential, we obtain

$$G(h, T) = \min_m F(m, h, T) \approx \min_m \left[\frac{1}{2}(k_B T - J)m^2 + \frac{k_B T}{12}m^4 + \dots - hm \right].$$

We thereby find that $F(m, h, T)$ recovers the behavior found from Weiss MFT, and specifically for $h = 0$ predicts a PM-FM phase transition at critical temperature $k_B T_c = J$, below which the convex $F(m, 0, T)$ (minimum at $m = 0$) becomes concave (with maximum at $m = 0$).

C. Variational mean-field theory

Another quite general approximate treatment is the variational mean-field theory, where the upper bound for the free energy, F is computed using a minimized variational free energy, F_{var} computed with a trial Hamiltonian, H_{tr} . To see how this upper bound is established we approximate the partition function,

$$\begin{aligned} Z &= \text{Tr} [e^{-H}] = \frac{1}{Z_{tr}} \text{Tr} [e^{-(H-H_{tr})} e^{-H_{tr}} e^{-F_{tr}}] = \langle e^{-(H-H_{tr})} \rangle_{tr} e^{-F_{tr}}, \\ &\geq e^{-\langle H-H_{tr} \rangle_{tr}} e^{-F_{tr}} \equiv e^{-F_{var}}, \end{aligned} \quad (58)$$

where the variational free energy

$$F_{var} = F_{tr} + \langle H - H_{tr} \rangle_{tr} \geq F,$$

provides the lower bound for the actual free energy, and H_{tr} is the trial Hamiltonian, with respect to which the above expectation value is computed. In above we used the convex property of the e^{-x} function to conclude that $\langle e^{-x} \rangle \geq e^{-\langle x \rangle}$.

The simplest trial Hamiltonian for the Ising model can be taken to be that of independent spins in an effective magnetic field, $H_{tr} = -g \sum_i \sigma_i$, with g treated as a variational parameter to be determined by minimizing the variational free energy, F_{var} over g .

D. Landau mean-field theory

In thinking about the deeper meaning of its derivation, I note that the implicit self-consistent MFT equation (41) for $m(B, T)$ is actually a saddle-point equation for the free-energy density $f(m, B, T)$ with respect to m , i.e., corresponds to $\partial f / \partial m = 0$. This allows one to compute $f(m, B, T)$ by integrating the saddle-point equation. While this can in principle be done exactly, this is unnecessary for our purposes here, as we are interested in the behavior near the critical point, where the magnetization is small, $m \ll 1$. Thus, Eq. (41) and Eq. (43) lead to a free energy that is quartic polynomial in the magnetization m , with a quadratic coefficient proportional to $1 - J_0/T$ and quartic one a positive constant.

While above mean-field analysis relies on a specific microscopic model, as was first argued by Lev D. Landau (1937), above mean-field predictions are much more universal and are a consequence of continuous phase transition. Guided by general symmetry principles, Landau postulated that near a continuous phase transition the free energy density exhibits a generic analytic expansion in powers of an order parameter, the magnetization, in the case of a PM-FM transition,

$$f = f_0 + \frac{1}{2}a(T)\mathbf{m}^2 + \frac{1}{4}b\mathbf{m}^4 + \dots - \mathbf{B} \cdot \mathbf{m}. \quad (59)$$

The form is dictated by the spin-rotational symmetry of the Hamiltonian for $\mathbf{B} = 0$ (for Ising case, $m \rightarrow -m$ is a symmetry for $B = 0$, dictating that no odd powers of m appear in $f(m)$), with coefficients smooth functions of T , and, crucially $a(T) = a_0(T/T_c - 1)$, changing sign to $a(T < T_c) < 0$.

As illustrated in the right part of Fig.6, in the Ising case for $a(T > T_c) > 0$, $f(m)$ is well-approximated by a parabola, with a single minimum at the origin, $m = 0$. In contrast, for $a(T < T_c) < 0$, the free energy develops a symmetric double-well form, minimized by a finite magnetization, $m = \sqrt{a/b} \sim |T - T_c|^{1/2}$. Indeed it is easy to verify that above Weiss mean-field theory exhibits this Landau form with specific coefficients $a(T)$, $b(T)$, etc. given by (43). Thus, this generic Landau theory indeed predicts the phenomenology near T_c found above.

I note that a new crucial ingredient arises for the case of a multi-component vector order-parameter, \mathbf{m} . While MFT exponents remain the same, as illustrated in left of Fig.6 the Landau free-energy potential, exhibits zero-energy (the so-called) Goldstone modes, corresponding to reorientation of the order parameter, that is, the motion along the minimum of the “Mexican hat” potential.

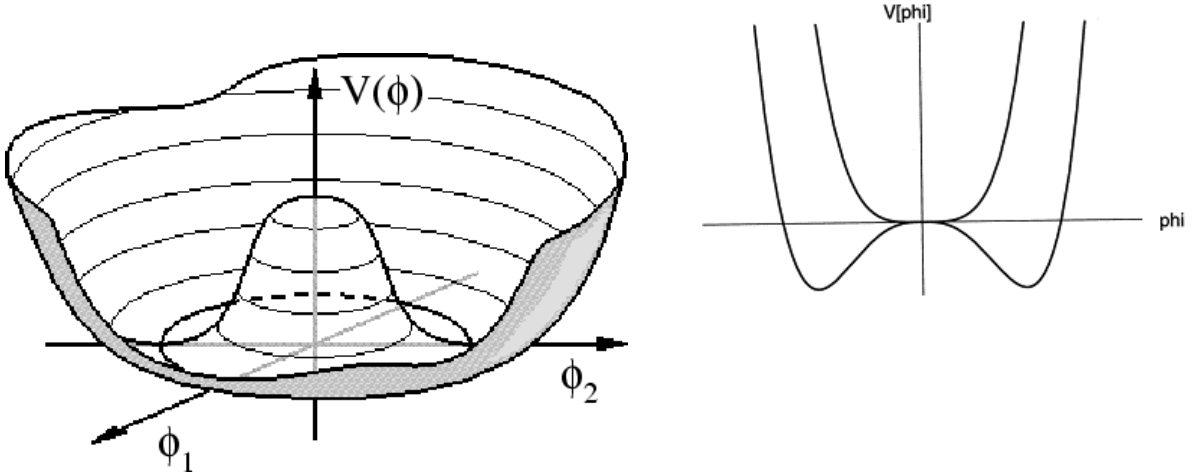


FIG. 6: A Mexican-hat potential and its cross-section controlling a continuous phase transition, illustrated for a two component order parameter $\Phi = (\phi_1, \phi_2)$ (e.g., the normal-to-superfluid or XY PM-FM). Massive (gapped) amplitude (Higg’s) and gapless Goldstone mode excitations respectively correspond to radial and azimuthal fluctuations about Φ_0 .

1. From Ising model to ϕ^4 field theory

As an illustration of a systematic treatment of a lattice model and alternative derivation of Ising mean-field theory, we study the classical the Ising model

$$H_{Ising} = -\frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} \sigma_i \sigma_j,$$

where $\sigma = \pm 1$ (representing spin up/down along z axis). The big advantage of the resulting continuum field theory is that it will be the starting point for beyond-MFT analysis, taking into account fluctuations, necessary particularly near a critical point.

While one can work directly with these Ising degrees of freedom σ_i , to expose the universal properties of this model, construct mean-field theory, study fluctuations and the associated PM-FM phase transition, it is much more convenient to transform this model to the so-called ϕ^4 field theory in terms of a continuous scalar field $\phi(\mathbf{r})$.

To this end we consider the partition function and manipulate it by introducing an auxiliary field ϕ_i , using a Hubbard-Stratonovich (HS) transformation (which, despite its “intimidating” name, is nothing more than a Gaussian integral from the calculus that we will develop on the homework and in the next lecture on phonon thermodynamics), which then allows us to execute the sum over $\{\sigma_i\}$ exactly, obtaining (see Gaussian calculus developed in the next lecture and on the homework),

$$Z = \sum_{\{\sigma_i\}} e^{\frac{1}{2}\beta \sum_{ij} J_{ij} \sigma_i \sigma_j}, \quad (60)$$

$$= Z_0^{-1} \sum_{\{\sigma_i\}} \int \mathcal{D}\phi_i e^{-\frac{1}{2}\beta^{-1} \sum_{ij} J_{ij}^{-1} \phi_i \phi_j + \sum_i \sigma_i \phi_i}, \quad (61)$$

$$= Z_0^{-1} \int \mathcal{D}\phi_i e^{-\frac{1}{2}\beta^{-1} \sum_{ij} J_{ij}^{-1} \phi_i \phi_j + \sum_i \ln \cosh \phi_i} \equiv \int \mathcal{D}\phi_i e^{-\beta H_{\text{eff}}(\phi_i)}. \quad (62)$$

In above, the inverse of a translationally-invariant exchange $J_{ij} \equiv J_{i-j}$ with Fourier transform $J(k)$ is straightforwardly inverted in Fourier space,

$$\sum_{ij} J_{ij}^{-1} \phi_i \phi_j = \int \frac{d^d k}{(2\pi)^d} \frac{1}{J(k)} \phi(-\mathbf{k}) \phi(\mathbf{k}).$$

For a short-range model, J_{i-j} is expected to be short-ranged and therefore with a Fourier transform that is well-defined at $J_{k=0}$ and falls off with increasing k beyond a short-scale microscopic length a . Thus, its generic form is given by

$$J(k) \approx \frac{J_0}{1 + (ka)^2}.$$

Combining this with H_{eff} , we obtain (dropping unimportant constant and going to a continuum limit $i = \mathbf{x}_i \rightarrow \mathbf{x}$)

$$H_{\text{eff}} = \frac{1}{2} \frac{(k_B T)^2}{J_0} \int_{\mathbf{k}} (1 + (ka)^2) \phi(-\mathbf{k}) \phi(\mathbf{k}) - k_B T a^d \int_{\mathbf{x}} \ln \cosh \phi(\mathbf{x}), \quad (63)$$

$$= \int_{\mathbf{x}} \left[\frac{1}{2} K (\nabla \phi)^2 + \frac{1}{2} \frac{(k_B T)^2}{J_0} \phi^2 - k_B T a^d \ln \cosh \phi(\mathbf{x}) \right], \quad (64)$$

where in the last line we went back to real (coordinate) space, took the continuum limit and defined the stiffness

$$K \equiv \frac{(k_B T)^2 a^{2-d}}{J_0}. \quad (65)$$

Above continuum theory of the Ising model can be straightforwardly analyzed within mean-field theory, by simply treating ϕ as spatially uniform (average magnetization), recovering mean-field results in our earlier Weiss mean-field analysis, and in particular predicting the PM-FM phase transition at T_c .

However, much more importantly, this model allows us to conveniently and systematically go beyond mean-field approximation by using the functional integral over $\phi(\mathbf{x})$, (62) to analyze the thermodynamics and the corresponding correlation and response functions. To make progress we note that near the PM-FM phase transition ϕ is small (fluctuating around zero in PM state and around a spontaneous small magnetization just below the transition inside the FM state). Thus we can Taylor expand the effective potential for ϕ to lowest nonlinear order,

$$\ln \cosh \phi(\mathbf{x}) = \ln 2 + \frac{1}{2} \phi^2 - \frac{1}{12} \phi^4 + O(\phi^6). \quad (66)$$

This then gives,

$$H_{\text{eff}} = H_{\text{Ising}}[\phi(\mathbf{x})] = \int_{\mathbf{x}} \left[\frac{1}{2} K (\nabla \phi)^2 + \frac{1}{2} t \phi^2 + \frac{1}{4} u \phi^4 \right], \quad (67)$$

where $\int_{\mathbf{x}} \equiv \int d^d x$, and we defined standard coupling constants of this effective Hamiltonian (often referred to as a ϕ^4 -theory or Ising field theory)

$$t = k_B T a^{-d} \left(\frac{k_B T}{J_0} - 1 \right), \quad u = k_B T a^{-d} / 3,$$

that (because of its generic nature) prominently appears in condensed matter and particle field theory studies. We note that the “reduced temperature”, t (not to be confused with time) is positive for $T > T_c \equiv J_0/k_B$, corresponding to a vanishing magnetization, $\phi = 0$ of

the PM phase and is negative for $T < T_c$, corresponding to a nonzero magnetization, $\phi > 0$ of the FM phase. Thus we this derivation is consistent with Weiss MFT, and therefore recovers the PM-FM phase transition at $t = 0$, corresponding to critical temperature $\sim J_0/k_B$.

Above scalar Landau ϕ^4 field model naturally generalizes from a single component Ising case of $N = 1$ (not to be confused with number of sites in the lattice model) to a general N . The result is an $O(N)$ model for N -component field $\vec{\phi}$ ($O(N)$ stands for orthogonal group of rotations, $\vec{\phi} \rightarrow R \cdot \vec{\phi}$ under which the model is invariant),

$$H_{O(N)}[\vec{\phi}(\mathbf{x})] = \int_{\mathbf{x}} \left[\frac{1}{2} K (\nabla \vec{\phi})^2 + \frac{1}{2} t |\vec{\phi}|^2 + \frac{1}{4} u |\vec{\phi}|^4 + \cdots - \vec{h} \cdot \vec{\phi} \right], \quad (68)$$

with XY ($O(N = 2)$) and Heisenberg ($O(N = 3)$) models. As we will explore in further lectures and on the homeworks, $N > 1$ case contains new important physics associated with “massless” Goldstone modes.

E. Beyond mean-field theory: critical phenomena and universality

Despite considerable success of Landau theory, it was appreciated as early as 1960s, that it fails qualitatively near most continuous phase transitions, and more general phenomenology is found in experiments, namely

$$M(T, B = 0) \propto |T_c - T|^\beta, \quad \chi(T) \propto |T - T_c|^{-\gamma}, \quad (69)$$

$$M(T = T_c, B) \propto B^{1/\delta}, \quad C(T) \propto |T - T_c|^{-\alpha}, \quad (70)$$

$$\xi(T_c, B = 0) \propto |T - T_c|^{-\nu}, \quad (71)$$

$$(72)$$

where “critical exponents” $\beta, \gamma, \delta, \alpha, \nu$ deviate from their MF values ($\beta_{\text{MF}} = 1/2, \gamma_{\text{MF}} = 1, \delta_{\text{MF}} = 3, \alpha_{\text{MF}} = 0, \nu_{\text{MF}} = 1/2$), are universal, depending only on the symmetry and dimensionality of the continuous phase transition, i.e., on its so-called “universality class”. They satisfy a variety of exact relations: $\alpha + 2\beta + \gamma = 2, \gamma = \beta(\delta - 1), d\nu = 2 - \alpha, \gamma = (2 - \eta)\nu$. In above we defined the correlation length ξ that characterizes the range of spatial correlations that diverge at the phase transition. A beautiful set of theoretical developments[21, 33] in the 1970s, led by M. Widom, Leo Kadanoff, Migdal, Michael Fisher, S. Pokrovsky, and Ken Wilson (who received the 1982 Nobel Prize for his development of renormalization group), led to a seminal explanation of experimental observations of universality and corrections to

Landau's mean-field theory. These arise due to qualitative and singular importance of fluctuations about mean-field predictions, a subject[21, 33] that we turn to in the next lecture on critical fluctuations and the renormalization group.

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