

Physics 7450: Solid State Physics 2

Lecture 4: Magnetism in charge insulators

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Abstract

In these lectures, we will study magnetism in insulators. After a warm up with paramagnetism of independent spins, we will discuss the spin exchange interactions in solids, arising from the combination of Coulomb repulsion and Pauli exclusion, and leads to the Heisenberg model of magnetism. Focussing on the simplest ferromagnetic and antiferromagnetic states, we will analyze thermodynamics and correlations of low-energy excitations around these states using Holstein-Primakoff and Schwinger bosons descriptions. We will use Jordan-Wigner transformation to solve a one-dimensional spin-1/2 chain. We will discuss coherent-spin states path-integral formulation of magnetism emphasizing, the role of Berry's phase and will analyze phase transitions using Landau's mean-field theory of FM and AFM phases.

I. INTRODUCTION

A. Outline

- Paramagnetism
- Spin exchange vs dipolar interaction
- Heisenberg model and crystalline anisotropies
- Hosten-Primakoff and Schwinger bosons
- Jordan-Wigner transformation and XXZ chain
- Coherent-spin states and Berry phases
- Mean-field and Landau theory of FM and AFM states

B. Background

In these notes we will explore some of aspects of magnetism in charge insulators. Magnetism is a formation and response of magnetic moments to external magnetic field $\mathbf{H}$ and their interaction. In general there are two sources of magnetic moment and associated magnetization density $\mathbf{M}$. One is quite intuitive, due to orbital charge current $\mathbf{j}$ in the material

$$\mathbf{M} = \frac{1}{2} \int_{\mathbf{r}} \mathbf{r} \times \mathbf{j},$$

much like current wire loop produces magnetic field. The other source is intrinsic electron spin $\mathbf{S}$, giving magnetization $\mathbf{M} = n\boldsymbol{\mu}$, where the magnetic moment is

$$\boldsymbol{\mu} = -\frac{g\mu_B}{\hbar}\mathbf{S},$$

where the g-factor $g \approx 2(1 + \frac{\alpha}{2\pi} + O(\alpha^2))$ (predicted by the Dirac equation with corrections beyond 2 coming from quantum electrodynamic fluctuations of the electromagnetic field, as an expansion in powers of the fine structure constant $\alpha = e^2/(4\pi\epsilon_0\hbar c) \approx 1/137$), $\mu_B = \frac{e\hbar}{2m} = 5.788 \times 10^{-5} eV/Tesla$ is Bohr magneton ($e > 0$ is proton's charge), and for the most part we will neglect nuclear spin since it leads to magnetism that is down by a factor of 2000 due to the electron-proton mass ratio.

The Hamiltonian for a single electron that predicts both orbital and spin magnetization is given by[1]

$$H = \frac{P^2}{2m} + V(\mathbf{r}) + \frac{e\hbar}{2m}\mathbf{s} \cdot \mathbf{B} + \frac{\hbar}{4m^2c^2}\boldsymbol{\sigma} \cdot \nabla V \times \mathbf{P} + \frac{\hbar^2}{8mc^2}\nabla^2 V + \frac{P^4}{8m^3c^2} + \dots, \quad (1)$$

where $\mathbf{P} = \mathbf{p} + e\mathbf{A}$ is the velocity operator that includes the electromagnetic vector potential, $V(\mathbf{r})$ is the scalar potential, and the subsequent terms are respectively the Zeeman term of spin-magnetic field interaction, spin-orbit interaction, Darwin term, and relativistic correction to the quadratic spectrum, all coming from the nonrelativistic limit of the Dirac equation (that can be obtained by squaring the Dirac Hamiltonian and expanding it at small velocities).

Expanding the kinetic energy term for a constant magnetic field in a gauge $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$, and neglecting higher order relativistic Darwin and p^4 terms, we obtain the simplified form

$$H = \frac{p^2}{2m} + V(\mathbf{r}) + \gamma(r)\boldsymbol{\ell} \cdot \mathbf{s} + \frac{\mu_B}{\hbar}(\boldsymbol{\ell} + 2\mathbf{s}) \cdot \mathbf{B} + \frac{e^2}{8m}(\mathbf{B} \times \mathbf{r})^2 \quad (2)$$

where $\gamma(r) = \frac{1}{2m^2c^2}\frac{1}{r}\frac{\partial V}{\partial r}$. This Hamiltonian captures the orbital and spin magnetism associated with a single electron and (appropriately generalized to many-electron system, which most importantly includes electron-electron Coulomb, crystal-field splitting and phonon interaction) is the starting point of the study of magnetic response of individual atoms, molecules and solids.

We note in passing that computing the classical partition function $Z(\mathbf{A})$ as a phase space integral $\int d^N\mathbf{r}d^N\mathbf{p}$ with a Boltzmann weight $e^{-\beta H[\mathbf{p}+e\mathbf{A},\mathbf{r}]}$, and shifting the integration variable from $\mathbf{p}$ to $\mathbf{P}$ allows us to eliminate all the orbital effects of the vector potential, illustrating that *orbital* magnetism is absent in classical physics and is an intrinsically quantum phenomenon, a result known as the Bohr-von Leeuwen theorem.

There is a lot of interesting and extensively studied physics associated with atomic and molecular magnetism, such as Larmor diamagnetism and van Vleck paramagnetism[1, 2]. However, here we instead focus on magnetism in solids.

II. ORIGIN OF MAGNETISM: COULOMB INTERACTION

As discussed in the Introduction, magnetism in solids arises from orbital and spin effects. In these set of notes we will first focus on local moment magnetism, valid for insulators,

leaving the treatment of itinerate magnetism for future lectures. For simplicity we focus on atomic states with finite total angular momentum $J > 0$, arising in partially filled atomic shells and spin-orbit interaction, with $\{J^2, J_z, L^2, S^2\}$ as the good atomic quantum numbers. In such systems the dominant term in the atomic Hamiltonian, (2), capturing the response to an external magnetic field is $H = \frac{\mu_B}{\hbar}(\boldsymbol{\ell} + 2\mathbf{s}) \cdot \mathbf{B}$, which when evaluated in the atomic eigenstates gives an effective $\mathbf{J}$ moment

$$\langle JLSJ_z | (\boldsymbol{\ell} + 2\mathbf{s}) | JLSJ_z \rangle = g_L(J, L, S) \langle JLSJ_z | \mathbf{J} | JLSJ_z \rangle,$$

where

$$g_L(J, L, S) = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

is the Landé g-factor, that leads to an effective Hamiltonian

$$H_{eff} = \frac{g_L \mu_B}{\hbar} \mathbf{J} \cdot \mathbf{B} \equiv -\boldsymbol{\mu} \cdot \mathbf{B}, \quad (3)$$

with $2J + 1$ eigenstates with eigenvalues $E_j = j g_L \mu_B B$, where $j \in \{-J, \dots, +J\}$.

A. Local moment paramagnetism

Armed with the effective $\mathbf{J}$ -moment Hamiltonian, (3), the magnetic linear susceptibility and other thermodynamic quantities as well as correlation functions are easily computed. As usual the thermodynamics is contained in the quantum partition function, that is a sum over $2J + 1$ discrete states projections of $\mathbf{J}$ along $\mathbf{B} = \mu_0 \mathbf{H}$, giving:

$$Z(H) = e^{-\beta F} = \sum_{j=-J}^J e^{-j g_L \mu_B B / k_B T} = \frac{\sinh[(J + 1/2) g_L \mu_B B / k_B T]}{\sinh[g_L \mu_B B / (2k_B T)]}, \quad (4)$$

The magnetization density

$$M = -n \partial F / \partial B = n g_L \mu_B J B_J(J g_L \mu_B B / k_B T), \quad (5)$$

where $B_J(x)$ is the Brillouin function, $B_J(x) = (1 + \frac{1}{2J}) \coth[(1 + \frac{1}{2J})x] - \frac{1}{2J} \coth(\frac{x}{2J}) \approx_{x \rightarrow 0} \frac{1}{3}(1 + 1/J)x$. For $J = 1/2$ (the so-called Ising case of $L = 0, S = 1/2$), $g_L = 2$ and magnetization reduces to $m = n \mu_B \tanh(\mu_B B / k_B T)$. For large J , the $2J + 1$ states can be equivalently treated as continuous magnetic moment orientation, integrating $\int d\Omega$ over the full 4π steradians of the solid angle orientations.

In the classical limit of $(J + 1/2)g_L\mu_B B \ll k_B T$, the result leads to Curie linear susceptibility (using $\coth x \approx 1/x + x/3 + \dots$)

$$\chi_C(H = 0, T) = \left. \frac{\partial M}{\partial B} \right|_{B \rightarrow 0} = \frac{1}{3} n (g_L \mu_B)^2 \frac{J(J+1)}{k_B T} \equiv \frac{C}{T},$$

with C the Curie constant and $M \approx \chi(T)B$ exhibiting a linear response in this regime. This $1/T$ susceptibility behavior is a generic experimental signature of independent local moments, with the amplitude 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 the field), only diverging at vanishing temperature, capturing a nonzero induced magnetization in response to an infinitesimal field in the absence of disordering thermal fluctuations. In the opposite quantum limit of large Zeeman gaps $(J + 1/2)g_L\mu_B B \gg k_B T$, magnetization density saturates at its maximum value of $ng_L J$. These limits are illustrated in Figs.(1) and (2). As we will see below in magnets, as a result of interactions between local moments, the behavior is far richer.

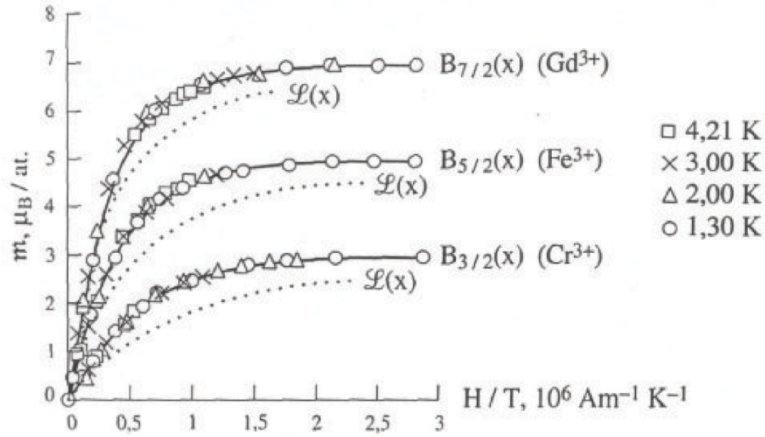


FIG. 1: Reduced magnetization curves for three paramagnetic salts and comparison with Brillouin theory prediction, from Ref.[1].

B. Spin-spin exchange interaction

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

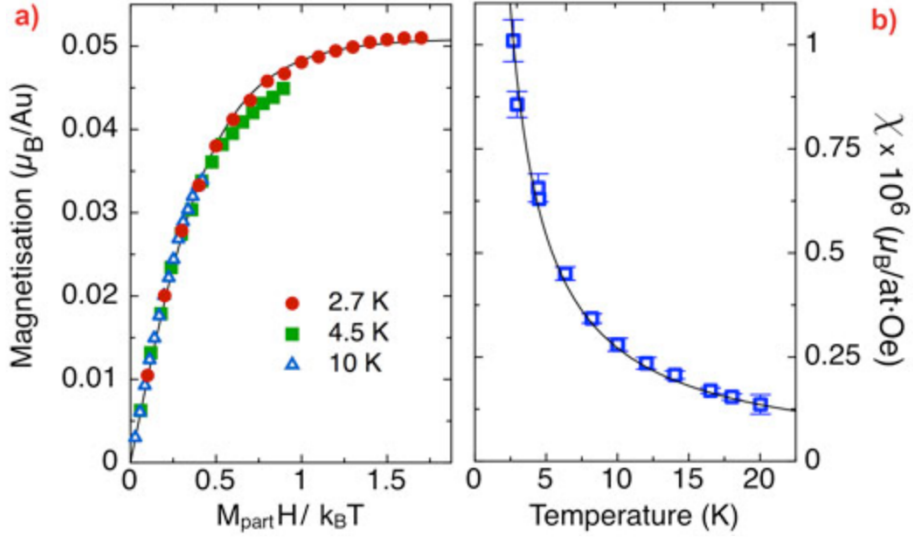


FIG. 2: Magnetization and corresponding Curie susceptibility in gold (Au) nanoparticles, measured at several temperatures up to $H = 17$ Tesla. Reduced magnetization curves for three paramagnetic salts and comparison with Brillouin theory prediction, from Ref.[3].

extends to magnetism with 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

$$H_{dipole-dipole} = \frac{\mu_0}{4\pi r^3} [\boldsymbol{\mu}_1 \cdot \boldsymbol{\mu}_2 - 3(\boldsymbol{\mu}_1 \cdot \hat{\mathbf{r}})(\boldsymbol{\mu}_2 \cdot \hat{\mathbf{r}})], \quad (6)$$

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 the measure of intermoment spacing between typical moments in a solid, an estimate of the dipole-dipole interaction energy is given by

$$E_{dipole-dipole} \approx \frac{\mu_0}{4\pi} \frac{\mu_B^2}{a_0^3} = \left(\frac{e^2}{4\pi\epsilon_0\hbar c} \right)^2 \frac{e^2}{16\pi\epsilon_0 a_0} \approx \left(\frac{1}{137} \right)^2 E_{Ry} \approx 5 \times 10^{-4} eV \approx \text{few Kelvin}, \quad (7)$$

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 it is spin-independent, as we will see below, it is the much larger (order of eV) Coulomb interaction that is responsible for magnetism in solids through its interplay with the Pauli principle, which brings spin configuration into the problem.

To see this we first examine Heitler-London (HL) theory of a covalent bond in e.g., a H_2 molecule, which one can think of as a toy model of two-site insulator. The system consists of two electrons and two nuclei (protons in H_2 case, assumed to be fixed classical degrees of freedom) on which electrons prefer to reside, characterized by hydrogenic-like exponentially localized wavefunction, $\psi_A(\mathbf{r}_1), \psi_B(\mathbf{r}_2)$. The corresponding Hamiltonian is $H(\mathbf{r}_1, \mathbf{r}_2) = H_A(\mathbf{r}_1) + H_B(\mathbf{r}_2) + H_{int}(\mathbf{r}_1, \mathbf{r}_2)$, where

$$H_A(\mathbf{r}_1) = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{e^2}{|\mathbf{r}_1 - \mathbf{R}_A|}, \quad H_B(\mathbf{r}_2) = -\frac{\hbar^2}{2m}\nabla_2^2 - \frac{e^2}{|\mathbf{r}_2 - \mathbf{R}_B|}, \quad (8)$$

$$H_{int}(\mathbf{r}_1, \mathbf{r}_2) = -\frac{e^2}{|\mathbf{r}_1 - \mathbf{R}_B|} - \frac{e^2}{|\mathbf{r}_2 - \mathbf{R}_A|} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \quad (9)$$

and single particle problems are defined by $H_{A,B}(\mathbf{r})\psi_A(\mathbf{r}) = \varepsilon_{A,B}\psi_{A,B}(\mathbf{r})$.

The HL assumption is that each electron predominantly resides on each ion, rather than being in the state of superposition between the two nuclei; thinking about a double-well potential problem, we note that in the absence of (or weak) interactions, it is this latter solution that is most natural, and can be thought of as a “toy” wavefunction of a complementary conductor.

However, a crucial point is that once we consider even a two-electron wavefunction, quantum statistics enters, Pauli principle requiring antisymmetry of the overall wavefunction under interchange of two electrons. Thus the full two-electron wavefunction (that for two particles breaks up into a product of orbital and spin parts) is given by $\Psi_{s,t}(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \psi_{s,t}(\mathbf{r}_1, \mathbf{r}_2)\chi_{s,t}(s_1, s_2)$, where the two singlet (s) and triplet (t) possibilities are

$$\begin{aligned} \psi_s(\mathbf{r}_1, \mathbf{r}_2) &= N_s [\psi_A(\mathbf{r}_1)\psi_B(\mathbf{r}_2) + \psi_A(\mathbf{r}_2)\psi_B(\mathbf{r}_1)], \quad \chi_s(s_1, s_2) = \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 - |\uparrow\rangle_2 |\downarrow\rangle_1], \\ \psi_t(\mathbf{r}_1, \mathbf{r}_2) &= N_t [\psi_A(\mathbf{r}_1)\psi_B(\mathbf{r}_2) - \psi_A(\mathbf{r}_2)\psi_B(\mathbf{r}_1)], \quad \chi_t(s_1, s_2) = |\uparrow\rangle_1 |\uparrow\rangle_2, \quad |\downarrow\rangle_1 |\downarrow\rangle_2, \\ &\quad \frac{1}{\sqrt{2}} [|\uparrow\rangle_1 |\downarrow\rangle_2 + |\uparrow\rangle_2 |\downarrow\rangle_1], \end{aligned} \quad (10)$$

where the singlet/triplet normalization factors are

$$N_{s,t} = \frac{1}{\sqrt{2(1 \pm |S_{AB}|^2)}}, \quad (11)$$

where $S_{AB} \equiv \int_{\mathbf{r}} \psi_A^*(\mathbf{r})\psi_B(\mathbf{r})d\mathbf{r}$.

The key observation is that despite spin-independence of Coulomb interaction its expectation value in these singlet and triplet states are quite different, given by

$$\varepsilon_s = \langle \psi_s | H | \psi_s \rangle = \varepsilon_A + \varepsilon_B + 2N_s^2(C + I), \quad (12)$$

$$\varepsilon_t = \langle \psi_t | H | \psi_t \rangle = \varepsilon_A + \varepsilon_B + 2N_t^2(C - I), \quad (13)$$

giving the single-triplet splitting energy

$$\Delta E_{s-t} \equiv 2J = \varepsilon_s - \varepsilon_t = 2(N_s^2 - N_t^2)C + 2(N_s^2 + N_t^2)I = 2\frac{C|S_{AB}|^2 - I}{1 - |S_{AB}|^4},$$

that is positive for

$$I < C|S_{AB}|^2,$$

where

$$C = \int_{\mathbf{r}_1, \mathbf{r}_2} \psi_A^*(\mathbf{r}_1)\psi_B^*(\mathbf{r}_2)H_{int}\psi_A(\mathbf{r}_1)\psi_B(\mathbf{r}_2) = \int_{\mathbf{r}_1, \mathbf{r}_2} n_A(\mathbf{r}_1)H_{int}n_B(\mathbf{r}_2), \quad (14)$$

$$I = \int_{\mathbf{r}_1, \mathbf{r}_2} \psi_A^*(\mathbf{r}_1)\psi_B^*(\mathbf{r}_2)H_{int}\psi_B(\mathbf{r}_1)\psi_A(\mathbf{r}_2), \quad (15)$$

are the *direct* (classical electrostatic part coming from density-density interaction) contribution of the interaction, and the *exchange integral* comes from quantum mechanical exchange of the two electrons, the existence of which was also independently pointed out by Heisenberg and Dirac in 1926.

The nontrivial exchange integral I that splits the singlet-triplet degeneracy arises from a nonvanishing overlap between the two wavefunctions localized on the A and B nuclei. For two electrons on a single atom $I > 0$ and gives the mechanism responsible for the Hund's rule of maximizing the total spin in a multi-electron atom. More generally I can be positive, *ferromagnetic* (FM) or negative, *antiferromagnetic* (AFM), but is found to be strongly negative for H_2 , showing that the molecule is in a spin-singlet state with the splitting responsible for H_2 binding. More importantly, above analysis thus illustrates the Coulomb-driven mechanism for magnetism in solids.

C. Heisenberg model

To flesh this out more explicitly, illustrating the significance of the exchange constant J , we illustrate that (when confined to the singlet $((\mathbf{s}_1 + \mathbf{s}_2)^2 = 0)$ — triplet $((\mathbf{s}_1 + \mathbf{s}_2)^2 = 2)$ subspace of two electrons) above splitting can be captured by a simple effective, pure spin Hamiltonian,

$$H_{eff} = \varepsilon_s + \frac{1}{2}(\varepsilon_t - \varepsilon_s)(\mathbf{s}_1 + \mathbf{s}_2)^2 = \varepsilon_s - J(\mathbf{s}_1 + \mathbf{s}_2)^2, \quad (16)$$

$$= \varepsilon_s - J(\mathbf{s}_1^2 + \mathbf{s}_2^2) - 2J\mathbf{s}_1 \cdot \mathbf{s}_2, \quad (17)$$

$$= -2J\mathbf{s}_1 \cdot \mathbf{s}_2 + E_0, \quad (18)$$

where $E_0 = \varepsilon_s - 3J/2$. H_{eff} is the famous Heisenberg Hamiltonian and we have taken spins to be dimensionless (absorbed $\hbar$ into J which then has dimensions of energy). When generalized for a lattice of “spins” $\mathbf{S}_i$ (a total localized angular momentum of an ion, that generally involves both orbital and spin angular momenta, with magnetic moment $\boldsymbol{\mu}_i = -g_L\mu_B\mathbf{J}_i$, but we will continue to use the standard notation of $\mathbf{S}_i$, and taking it to be dimensionless) at sites $\mathbf{R}_i$ of a solid with exchange J_{ij} between sites $\mathbf{R}_i$ and $\mathbf{R}_j$ it is given by

$$H = - \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j. \quad (19)$$

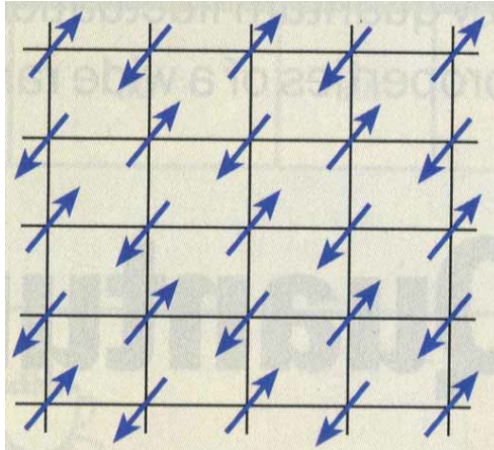


FIG. 3: Graphical determination of the mean-field magnetization M from the intersection points of the Brillouin function $B_S(x)$ and straight lines of temperature-dependent slope (figure by Solyom, Solids State Physics I).

In the quantum regime, this Hamiltonian is highly nontrivial (despite its deceptively simple quadratic form) as it is to be supplemented by the nonlinear spin commutation relation

$$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\epsilon_{\alpha\beta\gamma}S_i^\gamma.$$

We note that the ideal Heisenberg Hamiltonian has full $SU(2)$ spin-rotational invariance, with spin orientation totally independent of the orbital (e.g., bond) orientations. Below we will discuss deviation from this idealization due to spin-orbit interactions that result in the so-called crystal-symmetry and other $SU(2)$ symmetry-breaking fields. In the classical approximation, for $J > 0$ ($J < 0$) it predicts ferromagnetic (antiferromagnetic) alignment of spins at low temperature, that as we will see below leads to ferromagnets and antiferromagnets. Of course in the presence of quantum and thermal fluctuations the phenomenology is much richer and strongly depends on dimensionality of space and lattice structure. In the presence of an external magnetic field $\mathbf{H}$, with flux density $\mathbf{B} = \mu_0\mathbf{H}$ (that does *not* include magnetization due to local moments), there is an additional Zeeman interaction

$$H_{Zeeman} = -g\mu_B\mathbf{B} \cdot \sum_i \mathbf{S}_i,$$

($g \equiv -g_L$) that for strong fields can overwhelm the exchange, aligning all the moments along $\mathbf{B}$.

In addition to above direct *exchange* interaction, mediated by overlap between electron wavefunctions localized on neighboring ions, there are a number of other mechanisms that can lead to the effective Heisenberg model, even if direct exchange is absent. One is the *superexchange* mechanism put forward by H. A. Kramers (1934), where the spin interaction between magnetic atoms is mediated by electrons on the intermediate nonmagnetic atoms. Antiferromagnetism in certain fluorides (MnF_2 , CoF_2) and oxides (MnO , CuO) is believed to arise from this mechanism.

D. 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 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

$$H = - \sum_{i,j} J_{ij} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z).$$

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

$$H_{Ising} = - \sum_{i,j} J_{ij} S_i^z S_j^z.$$

Since only commuting S_i^z operators appear, in this Ising limit the model is classical 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 tranverse-field Ising (TFI) Hamiltonian

$$H_{TFI} = - \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z - \sum_i h_i \sigma_i^x,$$

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 $\hbar/2$ 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 .

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,

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

In addition, for $S > \hbar/2$, a single-ion anisotropy $H_{ion} = -D \sum_i (S_i^z)^2$ can also appear in tetragonal crystals.

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

$$H = - \sum_{i,j} J_{ij} \left(\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + \Delta S_i^z S_j^z \right). \quad (20)$$

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.

III. MAGNETISM IN CRYSTALLINE SOLIDS

Except for one-dimension (where it can be solved by Bethe Ansatz) the full quantum-mechanical Heisenberg model cannot be solved exactly. We thus embark on a variety of approximate analyses of this model, predicting appearance of variety of magnetic orders and phase transitions between them in crystalline solids.

A. Mean-field theory

The simplest and oldest approximate treatment of interacting systems in general is the so-called mean-field theory 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 deep in the classically well-ordered state, where fluctuations are small. In the context of magnetic system this is known as Weiss mean-field (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 theory on the Heisenberg model we assume the long-range magnetic order characterized by magnetization proportional to $\langle \mathbf{S}_i \rangle$, with spin then given by

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

the mean-field value and small fluctuations (presumed small). Inserting this into Heisenberg Hamiltonian in the presence of real external field and neglecting the small fluctuations terms

beyond first order, we obtain

$$H_{\text{mft}} = \sum_{i,j} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - 2 \sum_{i,j} J_{ij} \langle \mathbf{S}_j \rangle \cdot \mathbf{S}_i - g\mu_B \mathbf{B} \cdot \sum_i \mathbf{S}_i, \quad (21)$$

$$= \sum_{i,j} J_{ij} \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle - g\mu_B \mathbf{B}_{\text{eff}} \cdot \sum_i \mathbf{S}_i, \quad (22)$$

where the effective Weiss field is

$$\mathbf{B}_{\text{eff}} = \mathbf{B} + \frac{2}{g\mu_B} \sum_j J_{ij} \langle \mathbf{S}_j \rangle,$$

that quite clearly gives a self-consistent mechanism to induce magnetic order, $\langle \mathbf{S}_j \rangle \neq 0$ even for vanishing external magnetic field. Since above mean-field Hamiltonian, (22)lcoalPM is for a single spin, it can be solved exactly, as we will now do for a ferromagnetic order.

1. Ferromagnetic order

Focussing on the ferromagnetic state, we take $\langle \mathbf{S}_i \rangle \equiv \mathbf{S}_0 = \mathbf{M}\hbar/(g\mu_B)$ to be spatially uniform, which allows us to directly utilize our analysis from Sec.II A for Hamiltonian (22). From Eq.(5) we immediately find magnetization density along the applied field

$$M = ng_L\mu_B S B_S [Sg_L\mu_B B_{\text{eff}}(M)/k_B T], \quad (23)$$

$$= ng_L\mu_B S B_S [Sg_L\mu_B (B + \lambda M)/k_B T], \quad (24)$$

which gives a self-consistent equation for $M(B)$, with constant $\lambda = 2J_0/(ng_L^2\mu_B^2)$ and $J_0 \equiv \sum_j J_{ij}$ ($\approx Jz$ for nearest neighbors exchange model with z the lattice coordination number). This implicit equation can be solved graphically (or numerically), illustrated in Fig.??.

From its structure and

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

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

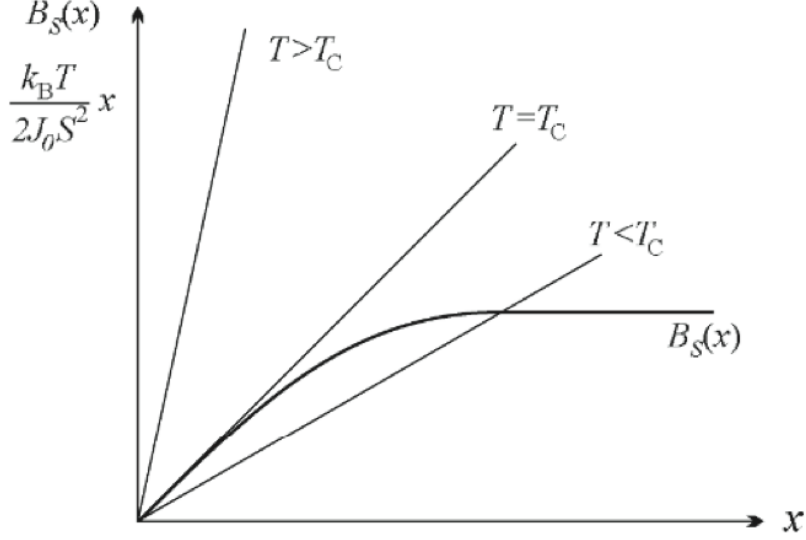


FIG. 4: Lattice of interacting spins (magnetic moments), exhibiting an antiferromagnetic (AFM) classical order (figure by Subir Sachdev).

the temperature at which the FM solution first appears and is given by

$$k_B T_c = \frac{1}{3} n g_L^2 \mu_B^2 S(S+1) \lambda, \quad (25)$$

$$= \frac{2J_0}{3} S(S+1) = \frac{2J_0}{3\hbar^2} \langle \mathbf{S}^2 \rangle. \quad (26)$$

quite naturally determined by the exchange constant J and square of the spin operator with larger spin ordering at higher temperature.

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

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

with the susceptibility

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

that (in contrast to the paramagnetic Curie susceptibility χ_C) diverges at $T_c > 0$, where the system exhibits paramagnetic (PM)-ferromagnetic (FM) continuous transitions. 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))

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

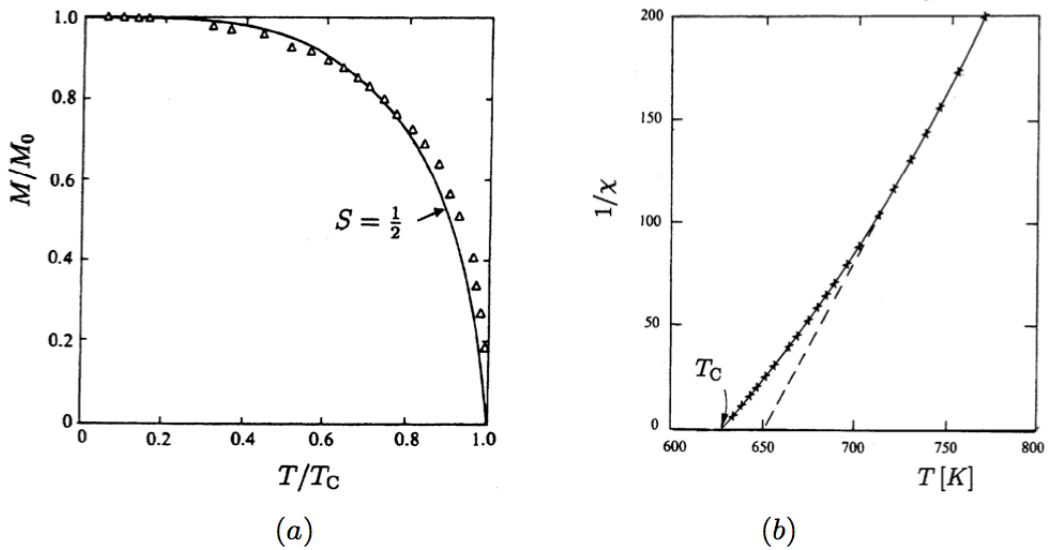


FIG. 5: Comparison of the measured magnetic properties of nickel [P. Weiss and R. Forrer, Ann. de Phys. 5, 153 (1926)] with the results obtained in the mean-field theory for $S = 1/2$. (a) Magnetization and (b) inverse susceptibility, as functions of temperature (figure from Solyom, Solids State Physics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

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 Neel or spin-density wave states.

2. Landau mean-field theory

While above mean-field analysis relies on a specific microscopic Heisenberg model, as was first demonstrated by Lev D. Landau (1937), above mean-field predictions are much more universal and are a consequence of continuous phase transition and a free-energy that is analytic function of the order parameter, magnetization in the case of the FM. Indeed Landau postulated that

$$F = F_0 + a(T)M^2 + \frac{1}{2}bM^4 + \dots - BM,$$

(with the form dictated by the spin-rotational [or at least $M \rightarrow -M$] symmetry of the Hamiltonian), with coefficients a smooth function of T and $a(T) = a_0(T/T_c - 1)$, changing

sign to $a(T < T_c) < 0$ at T_c . Indeed it is easy to verify that above Weiss mean-field theory indeed exhibits this Landau form with specific coefficients $a(T)$, $b(T)$, etc. Thus, this generic Landau theory indeed predicts the phenomenology near T_c found above.

3. From Ising model to ϕ^4 field theory

As an illustration of a systematic treatment of a lattice model we study the classical 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).

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 a the so-called $\phi - 4$ 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 Hubbard-Stratonovich (HS) transformation (which, despite its “scary” name, is nothing more than a Gaussian integral), which the allows us to execute the sum over $\{\sigma_i\}$ exactly, obtaining

$$Z = \sum_{\{\sigma_i\}} e^{\frac{1}{2}\beta \sum_{ij} J_{ij} \sigma_i \sigma_j}, \quad (27)$$

$$= Z_0^{-1} \sum_{\{\sigma_i\}} \int \mathcal{D}\phi_i e^{\frac{1}{2}\beta^{-1} \sum_{ij} J_{ij}^{-1} \phi_i \phi_j + \sum_i \sigma_i \phi_i}, \quad (28)$$

$$= Z_0^{-1} \int \mathcal{D}\phi_i e^{\frac{1}{2}\beta^{-1} \sum_{ij} J_{ij}^{-1} \phi_i \phi_j + \sum_i \ln \cosh \phi_i} \equiv \int \mathcal{D}\phi_i e^{-H_{eff}(\phi_i)}. \quad (29)$$

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,

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

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 $i = \mathbf{r}_i \rightarrow \mathbf{r}$)

$$H_{eff} = \frac{1}{2} \frac{k_B T}{J_0} \int_{\mathbf{k}} (1 + (ka)^2) \phi(-\mathbf{k}) \phi(\mathbf{k}) - a^d \int_{\mathbf{r}} \ln \cosh \phi(\mathbf{r}), \quad (30)$$

$$= \int_{\mathbf{r}} \left[\frac{1}{2} K (\nabla \phi)^2 + \frac{1}{2} \frac{k_B T}{J_0} \phi^2 - a^d \ln \cosh \phi(\mathbf{r}) \right], \quad (31)$$

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

$$K \equiv \frac{k_B T a^{2+d}}{J_0}.$$

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 early Weiss mean-field analysis, and in particular predicting the PM-FM phase transition at T_c .

However, this model also allows us to conveniently go beyond mean-field by using the functional integral over $\phi(\mathbf{r})$ to analyze the thermodynamics via above partition function. To make progress we note that near the PM-FM phase transition ϕ is small (fluctuating around zero in PM state and around spontaneous small magnetization just below the transition inside the FM state). Thus we can Taylor expand the effective ϕ potential to lowest nonlinear order,

$$\ln \cosh \phi(\mathbf{r}) = \ln 2 + \frac{1}{2} \phi^2 - \frac{1}{12} \phi^4 + O(\phi^6). \quad (32)$$

This then gives,

$$H_{eff} = \int_{\mathbf{r}} \left[\frac{1}{2} K (\nabla \phi)^2 + \frac{1}{2} t \phi^2 + \frac{1}{4!} u \phi^4, \right] \quad (33)$$

where we defined standard coupling constants of this effective Hamiltonian, often referred to as ϕ^4 -theory

$$t = a^d \left(\frac{k_B T}{J_0} - 1 \right), \quad u = 2a^d,$$

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 the theory recovers a PM-FM phase transition at $t = 0$, corresponding to critical temperature J_0/k_B .

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

Despite considerable success of Landau theory, it was appreciated as early as 1960s, that for continuous transitions a more general phenomenology is found in experiments, namely

$$M(T, B = 0) \propto |T_c - T|^\beta, \quad \chi(T) \propto |T - T_c|^{-\gamma}, \quad (34)$$

$$M(T = T_c, B) \propto B^{1/\delta}, \quad C(T) \propto |T - T_c|^{-\alpha}, \quad (35)$$

$$\xi(T_c, B = 0) \propto |T - T_c|^{-\nu}, \quad (36)$$

$$(37)$$

where “critical exponents” $\beta, \gamma, \delta, \alpha, \nu$ are universal, depending only on the symmetry and dimensionality of the continuous phase transition, namely the so-called its “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 mean-field theory $\beta = 1/2, \gamma = 1, \delta = 3, \alpha = 0, \nu = 1/2$, but more generally are irrational but universal numbers. 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[2, 14] in the 1970s, led by M. Widom, Leo Kadanoff, Migdal, Michael Fisher, S. Pokrovsky, and Ken Wilson (who received the 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[2, 14] that we will not pursue further here as it lies outside of our main focus.

IV. EXCITATIONS IN MAGNETIC STATES

The nature of the magnetic state depends strongly on the microscopic details such as the exchange interactions J_{ij} (its sign and range) and crystal lattice structure. One of important characterizations of a phase is its excitations, that strongly depend on the type of magnetic order (FM, AFM, spin-density wave, etc.). This is quite analogous to the phonon excitations in the ordered crystalline phase, and to zero-sound Bogoliubov excitations in the superfluid state, that we studied in previous chapters. Excitations in the magnetic ordered states are characterized by precessional spin dynamics, that in the classical limit is simply given by the torque equation $d\mathbf{I}/dt = \boldsymbol{\mu} \times \mathbf{B}$ for the local angular momentum $\mathbf{I}_i = \hbar \mathbf{S}_i$ of the local moment

$\boldsymbol{\mu} = -g_L\mu_B\mathbf{S}_i/\hbar$, and leads to collective spin-wave excitations. Quantum mechanically this is equivalent to the Heisenberg equation of motion for the spin operator $\mathbf{S}_i$, governed by the Heisenberg Hamiltonian,

$$i\hbar\frac{d\mathbf{S}_i}{dt} = [\mathbf{S}_i, H] = i\mathbf{S}_i \times \left(2\sum_j J_{ij}\mathbf{S}_j\right), \quad (38)$$

where in the second equality we used spin algebra to evaluate the commutator, obtaining precessional dynamics of each spin in the effective field of its neighbors. In analogy with lattice vibrations that in a quantum treatment led to quantized phonon excitations, magnetic spin-waves are treated fully quantum-mechanically. As we will see below this leads to magnetic excitation quanta referred to as magnons. Below we focus on the simplest homogeneous FM state and refer the reader for to the literature (see e.g.,[2] for the description of other states.

A. Ferromagnetic spin-waves

Focussing on the FM state, we study the dynamics of small spin fluctuations, $\delta\mathbf{S}_i = \mathbf{S}_i - \mathbf{S}_0$ (not unlike Goldstone modes phonon fluctuations as small distortions of the ordered state) about the average, spatially uniform mean magnetization $\mathbf{S}_0$ of the FM state. These are governed by linearized Heisenberg equation

$$\hbar\frac{d\delta\mathbf{S}_i}{dt} = 2\sum_j J_{ij} [\delta\mathbf{S}_i \times \mathbf{S}_0 + \mathbf{S}_0 \times \delta\mathbf{S}_j], \quad (39)$$

$$= 2\sum_j J_{ij} [\delta\mathbf{S}_i - \delta\mathbf{S}_j] \times \mathbf{S}_0, \quad (40)$$

that is decoupled in terms of Fourier components

$$\delta S_i^x = \delta S_k \cos(\mathbf{k} \cdot \mathbf{R}_i - \omega_k t), \quad \delta S_i^y = \delta S_k \sin(\mathbf{k} \cdot \mathbf{R}_i - \omega_k t),$$

giving the dispersion

$$\hbar\omega_{\mathbf{k}} = 2S_0 \sum_j J_{ij} [1 - e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_i)}] \sim Kk^2, \quad (41)$$

In the last equality we focussed on long-wavelength and utilized inversion symmetry of the lattice, that gives $K = \frac{2S_0}{d} \sum_R J_R R^2$ obtaining a *quadratic* (cf linear phonons) dispersion, that is a well-known signature of the ferromagnetic spin waves.

B. Antiferromagnetic spin-waves

A similar analysis to the above can be carried out for the AFM, with the key difference being the nature of the ordered state, characterized by a spatially oscillatory magnetization

$$\langle \mathbf{S}_i \rangle = S_0 e^{i\mathbf{k}_0 \cdot \mathbf{R}_i},$$

rather than the uniform one of a FM. Focussing on the commensurate Neel state, that only doubles the crystal's unit cell, with $2k_0 = 2\pi/a$, the corresponding equations can be straightforwardly solved, giving

$$\hbar\omega_k = 2S\sqrt{[J(\mathbf{k}_0) - J(\mathbf{k})][J(\mathbf{k}_0) - J(\mathbf{k} - \mathbf{k}_0)]},$$

where $J(\mathbf{k}) = \sum_j J_{ij} e^{i\mathbf{k} \cdot (\mathbf{R}_j - \mathbf{R}_i)}$. On a bipartite lattice (each lattice site can be unambiguously assigned to one of two sublattices), $J(\mathbf{k}_0) = zJ$ and $J(\mathbf{k} - \mathbf{k}_0) = -J(\mathbf{k})$ (z coordination number), the frequency reduces to

$$\hbar\omega_{\mathbf{k}} = 2S_0 z J \sqrt{1 - \gamma_{\mathbf{k}}^2} \sim ck,$$

where $\gamma_{\mathbf{k}} = \frac{1}{z} \sum_{\delta_j} e^{i\mathbf{k} \cdot \delta_j}$ and in the last equality we specialized to a long wavelength limit, obtaining the characteristic linear dispersion of the AFM spin waves.

C. Quantum treatment of ferromagnetic excitations: magnons

Following our earlier treatments of ordered states and excitations about them, we now study magnetic states in a fully quantum mechanical treatment. We first observe that a fully polarized FM state, $|FM\rangle \equiv |0\rangle = |-S, -S, \dots, -S\rangle$, with every spin having the same maximum projection $-S$ (or equivalently $+S$) along the same z -axis is an exact eigenstate of the Heisenberg Hamiltonian. This is obvious from the (20) form since S_i^- annihilates a fully polarized state, $|0\rangle$ (and S_i^+ annihilates $|NS\rangle$ FM state) and $S_i^z S_j^z$ leads to $E = -\sum_{ij} J_{ij} S^2$ eigenvalue. For a ferromagnetic interaction, this fully polarized FM state is the ground state. This state is degenerate with $2NS + 1$ other fully polarized states generated by acting on FM state by $1/\sqrt{N} \sum_i S_i^+$, corresponding to FM state with a rotated quantization axis but same $\mathbf{S}_{tot}^2 = NS(NS + 1)$ eigenvalue.

Excited state are produced by flipping spins locally, applying a string of S_i^+ , though in general this is not an eigenstate of the Heisenberg Hamiltonian as $S_j^+ S_i^-$ component will

move such excitations from site i to j . This is not surprising for a translationally invariant Hamiltonian, where a single spin excitation is an eigenstate of linear momentum, given by

$$|\psi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{2SN}} \sum_{\ell} e^{i\mathbf{k}\cdot\mathbf{R}_{\ell}} S_{\ell}^{+} |0\rangle \equiv a_{\mathbf{k}}^{\dagger} |0\rangle.$$

Above we defined $a_{\mathbf{k}}^{\dagger}$ as the single magnon creation operator, that is nearly bosonic, satisfying

$$[a_{\mathbf{k}}, a_{\mathbf{k}'}^{\dagger}] = -\frac{1}{2SN} \sum_{\ell} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_{\ell}} 2S_{\ell}^z \approx \delta_{\mathbf{k},\mathbf{k}'},$$

nearly fully saturated state $S_{\ell}^z \approx -S$. In real space we then have for nearly saturated FM state with large S ,

$$S_i^{+} = \sqrt{2S} a_i^{\dagger}, \quad S_i^{-} = \sqrt{2S} a_i, \quad S_i^z = -S + a_i^{\dagger} a_i. \quad (42)$$

Applying Heisenberg Hamiltonian operator to this state, it is straightforward to show[2] that its eigenvalue is given by $E_k = E_0 + 2S \sum_j J_{ij} [1 - e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}] - g\mu_B\mu_0 H$, where E_0 is the eigenvalue of the $|0\rangle$ state and we have added an external magnetic field $\mathbf{H} = H\hat{\mathbf{z}}$. For the FM exchange and/or in the presence of a large external field, the latter is the ground state and the single magnon excitation energy is given by (41) found from the Heisenberg equation of motion. For nearest-neighbors FM exchange on a 3d cubic lattice, we find

$$\hbar\omega_{\mathbf{k}} = 2JSz(1 - \gamma_{\mathbf{k}}), \quad (43)$$

$$= 4dJS \sum_{\delta_i} (1 - e^{i\mathbf{k}\cdot\delta_i}), \quad (44)$$

$$\begin{aligned} &= 2JS(6 - 2\cos k_x a - 2\cos k_y a - 2\cos k_z a) = 8JS \left(\sin^2 \frac{k_x a}{2} + \sin^2 \frac{k_y a}{2} + \sin^2 \frac{k_z a}{2} \right), \\ &\approx (2JSa^2)k^2. \end{aligned} \quad (45)$$

D. Holstein-Primakoff, Schwinger bosons and Jordan-Wigner fermion representations

1. Holstein-Primakoff representation

As we saw above, single spin-flip magnon excitations of a fully polarized and large S state is well described by approximately bosonic excitations, summarized in Eq.(42). There

in fact exists a rigorously exact bosonic representation in fact exists as first introduced by Holstein and Primakoff[6]

$$S_i^+ = a_i^\dagger(2S - a_i^\dagger a_i)^{1/2}, \quad S_i^- = (2S - a_i^\dagger a_i)^{1/2} a_i, \quad S_i^z = -S + a_i^\dagger a_i, \text{ with } 0 \leq a_i^\dagger a_i \leq 2S. \quad (46)$$

With the bosonic commutation relations of $a, a^\dagger$, it is straightforward to show that these spin operators exactly satisfy the spin algebra, e.g., $[S_i^+, S_i^-] = 2S_i^z$, with square-roots ensuring a $2S + 1$ -dimensional Hilbert space for spin S . To lowest order in the expansion of the square-root (valid for large S and for a highly polarized state), these reduce the approximate expressions, (42). Higher order terms generate magnon interactions.

Ferromagnet:

Expression the Heisenberg Hamiltonian in an external field $h \equiv g\mu_B B \hat{\mathbf{z}}$ to lowest order in terms of the Holstein-Primakoff bosons we find

$$H = - \sum_{i,j} J_{ij} \left(\frac{1}{2} S_i^+ S_j^- + \frac{1}{2} S_i^- S_j^+ + \Delta S_i^z S_j^z \right) - h \sum_i S_i^z, \quad (47)$$

$$\approx - \sum_{i,j} J_{ij} \Delta S^2 + S \sum_{ij} J_{ij} \left(\Delta a_i^\dagger a_i + \Delta a_j^\dagger a_j - a_i^\dagger a_j - a_j^\dagger a_i \right) - h \sum_i \left(-S + a_i^\dagger a_i \right), \quad (48)$$

$$\approx E_0 + S \sum_{ij} J_{ij} \left(a_i^\dagger a_i + a_j^\dagger a_j - a_i^\dagger a_j - a_j^\dagger a_i \right) - \mu_h \sum_i a_i^\dagger a_i + H_{int}, \quad (49)$$

$$\approx E_0 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + H_{int} \quad (50)$$

where $E_0 = - \sum_{ij} J_{ij} \Delta S^2 + hS$ is the ground state energy, $\mu_h = h - 2S \sum_j J_{ij} (\Delta - 1)$ the effective magnon chemical potential coupling to conserved total $S_{tot}^z = \sum_i S_i^z$ and

$$\hbar \omega_{\mathbf{k}} = 2S \sum_{\delta} J_{\delta} [1 - e^{i\mathbf{k} \cdot \delta}] - \mu_h \approx K k^2 - \mu_h,$$

the corresponding magnon dispersion in agreement with that found by other methods above. For a dilute gas of magnons we can neglect magnon interactions

$$H_{int} \approx - \sum_{ij} J_{ij} \left(a_i^\dagger a_i a_j^\dagger a_j - \frac{1}{2} a_i a_j^\dagger a_j^\dagger a_j - \frac{1}{2} a_i^\dagger a_i a_i a_j^\dagger \right)$$

and treat them as independent bosons, much like for the phonons and Bogoluibov quasi-particles of previous lectures. For high density of magnons interaction becomes important and can be treated by a variety of methods like perturbation theory, Hartree mean-field

theory (as in our Bogoluibov approximation for the Bose gas), etc. The interaction leads to a temperature-dependent correction to the magnon k^2 dispersion and more importantly generates an imaginary part that corresponds to a finite magnon lifetime, with a decay rate proportional to k^4 . The interaction also leads to a two-magnon bound state as rigorously studied by Dyson (1956).

Antiferromagnet:

Holstein-Primakoff bosons can also be used to study excitations in the Néel state as the approximate ground state of an AFM for $J < 0$. Since Néel state doubles the period of the underlying lattice, it must be treated as two magnetic sublattice sites A (spin up) and B (spin down), with two distinct Holstein-Primakoff expansions about $\pm S$ polarized states, respectively.

Focusing for simplicity on a nearest neighbor exchange model on a cubic lattice, the resulting Hamiltonian of excitations takes a Bogoluibov form,

$$H_{AFM} \approx 2NzJS^2 - 2JS \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left(a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + b_{\mathbf{r}'}^\dagger b_{\mathbf{r}'} + a_{\mathbf{r}} b_{\mathbf{r}'} + b_{\mathbf{r}'}^\dagger a_{\mathbf{r}}^\dagger \right). \quad (51)$$

Diagonalizing this Hamiltonian on a 3d cubic lattice using Bogoluibov (symplectic) transformation

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, \quad \beta_{\mathbf{k}} = u_{\mathbf{k}} b_{-\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}^\dagger,$$

obtaining

$$H = E_{gs} + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left[\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \right],$$

we can find the the ground state energy $E_{gs} = 2NzJS(S+1) + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}}$, that includes the mean-field energy of the Néel state and the zero-point quantum fluctuations, the coherence factors

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left[(1 - \gamma_{\mathbf{k}}^2)^{-1/2} + 1 \right], \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left[(1 - \gamma_{\mathbf{k}}^2)^{-1/2} - 1 \right], \quad (52)$$

and the spectrum

$$\hbar \omega_{\mathbf{k}} = 2|J|zS \left(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 + 2\gamma_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} \right), \quad (53)$$

$$= 2|J|zS \sqrt{1 - \gamma_{\mathbf{k}}^2}, \quad (54)$$

$$\approx (2\sqrt{2}|J|za)k \equiv c_{afm}k, \quad (55)$$

showing that at small ka the AFM spectrum is linear in k (as opposed to k^2 in a FM) with speed of magnon sound c_{afm} .

Because of quantum fluctuations in the ground state (since Néel state is not a true ground state of Heisenberg Hamiltonian), even a $T = 0$ expectation value of spin projection $\langle AFM | S_i^z | AFM \rangle$ is reduced from its fully polarized $\pm S$ value, by

$$\delta S = \frac{2}{N} \sum_{\mathbf{k}} \langle AFM | a_{\mathbf{k}}^\dagger a_{\mathbf{k}} | AFM \rangle = \frac{1}{N} \sum_{\mathbf{k}} [(1 - \gamma_{\mathbf{k}}^2)^{-1/2} - 1], \quad (56)$$

in analogy with the condensate depletion by interactions in the Bogoliubov theory of weakly interacting superfluid. The actual value depends on the dimensionality, type of a lattice, and exchange J_{ij} . The result can be straightforwardly generalized to finite temperature, as in condensate depletion in superfluids.

2. Schwinger bosons

An alternative and a more convenient representation of spin operators is in terms of “Schwinger bosons”, [7], that is a spinor bosonic operator

$$z^\dagger = (z_1^\dagger, z_2^\dagger),$$

with two flavors of bosons on each lattice site, $[z_\alpha, z_\beta^\dagger] = \delta_{\alpha\beta}$. The Schwinger boson structure is very intuitive with S_z component counting the difference between two flavors of bosons and spin raising and lowering operators naturally converting between the two flavors of Schwinger bosons,

$$\mathbf{S} = \frac{1}{2} z^\dagger \boldsymbol{\sigma} z = \frac{1}{2} z_\alpha^\dagger \boldsymbol{\sigma}_{\alpha\beta} z_\beta, \quad (57)$$

$$S_z = \frac{1}{2} (z_1^\dagger z_1 - z_2^\dagger z_2), \quad S^+ = z_1^\dagger z_2, \quad S^- = z_2^\dagger z_1, \quad (58)$$

with spin raising/lowering operators change the number difference, $n_1 - n_2$ of the two types of bosons, but preserves the total number of bosons, $n_1 + n_2 = 2S$. The spin-rotational invariance is implemented via SU(2) transformation $z \rightarrow Uz$,

$$U_{\hat{\mathbf{n}}} = e^{i\phi S_z/\hbar} e^{i\theta S_x/\hbar} e^{i\chi S_z/\hbar}, \quad (59)$$

that corresponds to SO(3) orthogonal rotation, $\mathbf{R}$ of the spin $\mathbf{S} \rightarrow \mathbf{R}\mathbf{S}$, with

$$R_{ij} S_j = \frac{1}{2} z_\gamma^\dagger U_{\gamma\alpha}^\dagger \sigma_{\alpha\beta}^i U_{\beta\delta} z_\delta,$$

corresponding to rotation of the $\hat{\mathbf{z}} \rightarrow \hat{\mathbf{n}}$, latter defined by Euler angles θ, ϕ, χ . $SU(2)$ algebra is $2^2 - 1 = 3$ dimensional (three angles), but angle χ spanning $U(1)$ subgroup of $SU(2)$ clearly does not enter $\mathbf{S}$, so the orbit space spanned by unit vector $\hat{\mathbf{n}}$ is a surface of a sphere $S^2 = SU(2)/U(1)$.

The spin components satisfy spin commutation relations,

$$[S_i^z, S_i^\pm] = \pm S_i^\pm, \quad [S_i^+, S_i^-] = 2S_i^z.$$

and the constraint $\mathbf{S}^2 = S(S+1)$ with $S = \frac{1}{2}z^\dagger z = \frac{1}{2}(z_1^\dagger z_1 + z_2^\dagger z_2)$. This constraint introduces an effective hard-core interactions for Schwinger bosons, that if formally eliminated (by solving for one of the bosons in terms of the other) gives back the Holstein-Primakoff representation.

To demonstrate above it is useful to take advantage of the following identity of Pauli matrices:

$$\boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta} = -\delta_{\alpha\beta}\delta_{\gamma\delta} + 2\delta_{\alpha\delta}\delta_{\beta\gamma}$$

3. $S=1/2$ hard-core boson representations

Another convenient representation for spin-1/2 is in terms of the so-called “hard-core” bosons. As we saw in our discussion of Holstein-Primakoff representation one had to introduce square-root factors to limit the bosonic Hilbert space to $2S+1$ and to encode the spin algebra in terms of bosonic commutation relations. However, for $S = 1/2$, this can be more simply done by the following identification:

$$|S = -1/2\rangle \rightarrow |n = 0\rangle, \quad |S = 1/2\rangle \rightarrow |n = 1\rangle, \quad (60)$$

$$S^+ = a^\dagger, \quad S^- = a, \quad S^z = a^\dagger a - 1/2 = n - 1/2, \quad (61)$$

$$[S^-, S^+] = -2S^z \rightarrow [a^\dagger, a] = -(2n - 1), \quad (62)$$

together with a hard-core constraint limiting bosonic states to $|n = 0\rangle, |n = 1\rangle$. The latter can be implemented by strong on-site interaction $H_{int} = U \sum_i (n_i^2 - n_i)$ in the limit of $U \rightarrow \infty$, hence “hard-core”.

With this the Heisenberg model reduces to:

$$H = - \sum_{i,j} J_{ij} \left(a_i^\dagger a_j + \Delta(n_i n_j - 2n_i) \right) - h \sum_i n_i, \quad (63)$$

with an implicit hard-core constraint, of $n_i = 0, 1$.

4. $S=1/2$ Jordan-Wigner fermion representations

For spin-1/2, the spin algebra and hard-core constraint can be more simply implemented by the use of fermionic spinor representation $c_\alpha = (c_\uparrow, c_\downarrow)$, associating the two states with the “magnetization”. The constraint can equivalently be implemented by a single spinless fermionic species with $S_z = \pm 1/2$ automatically implemented through Pauli principle corresponding fermionic occupation of 0 and 1. In 1d a powerful Jordan-Wigner (spinless) fermion representation exists,

$$S_i^+ = c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j}, \quad S_i^- = e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i, \quad S_i^z = c_i^\dagger c_i - \frac{1}{2}. \quad (64)$$

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,

$$[S_i^+, S_i^-] = c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j} e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i - e^{-i\pi \sum_{j<i} c_j^\dagger c_j} c_i c_i^\dagger e^{i\pi \sum_{j<i} c_j^\dagger c_j}, \quad (65)$$

$$= c_i^\dagger c_i - c_i c_i^\dagger = 2(n_i - 1/2) = 2S_z. \quad (66)$$

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

$$[S_i^+, S_j^-] = c_i^\dagger e^{i\pi \sum_{k<i} c_k^\dagger c_k} e^{-i\pi \sum_{l<j} c_l^\dagger c_l} c_j - e^{-i\pi \sum_{l<j} c_l^\dagger c_l} c_j c_i^\dagger e^{i\pi \sum_{k<i} c_k^\dagger c_k}, \quad (67)$$

$$= c_i^\dagger c_j e^{i\pi \sum_{k<i} c_k^\dagger c_k} e^{-i\pi \sum_{l<j} c_l^\dagger c_l} + c_j c_i^\dagger e^{-i\pi \sum_{l<j} c_l^\dagger c_l} e^{i\pi \sum_{k<i} c_k^\dagger c_k} = 0, \quad (68)$$

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

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

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_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.

E. Magnon thermodynamics in a ferromagnetic state

In this dilute magnon gas approximation (valid at low T and well polarized state), we can compute the corresponding thermodynamics of a ferromagnet.

The magnetization $M = V^{-1}g\mu_B \langle S_{tot}^z \rangle$ is well described

$$\langle S_{tot}^z \rangle = -NS + \sum_i \langle a_i^\dagger a_i \rangle = -NS + \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle, \quad (69)$$

$$= -NS + V \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}} - 1}, \quad (70)$$

where the correction to the fully polarized value is due to thermally excited magnons and those created by an external field. There is an obvious close analogy of BEC to the fully polarized state $|0\rangle$ and thermally excited magnons as condensate depletion. We note however, that in contrast, here there are no anomalous magnon terms, encoding the absence of any fluctuations in the ferromagnetically ordered state. Furthermore, the dispersion here is quadratic rather than linear of the phonons.

In the absence of anisotropy and external field $h = 0$, the density of thermally excited magnons is easily computed and in 3d given by the well-confirmed Bloch law $(k_B T/K)^{3/2}$, that gives how magnetization is thermally suppressed. Heat capacity is also straightforwardly computed as the temperature derivative of the energy $E = \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$, which in 3d gives

$$C_{FM} \sim (k_B T/2JS)^{3/2},$$

that contrasts from the acoustic phonon result that is T^d , i.e., T^3 in 3d.

The finite temperature magnetic response is also found by computing the increased number of magnons (that reduce magnetization) with increasing external magnetic field

$$M(H) = -M_0 + g\mu_B \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}(H)} - 1} - g\mu_B \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}(H=0)} - 1}, \quad (71)$$

$$\approx -M_0 + g\mu_B \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta(Kk^2 + \gamma H)} - 1} - g\mu_B \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{\beta Kk^2} - 1}, \quad (72)$$

At vanishing magnetic field H and isotropic model, we find $M \sim H^{1/2}$, that contrasts qualitatively from the constant longitudinal susceptibility, $M = \chi_{mft}^L H$ found in mean-field theory.

F. Antiferromagnetic ground state and its excitations

For negative exchange constant $J < 0$ it is clear that neighboring spins want to anti-align. This is a reflection of the tendency of two spins (as we saw in London-Heitler theory of H_2 molecule) to form a single state. A natural classical ground state is the Néel state where spins alternate $\pm S$ on A and B sublattices of a bipartite lattice, $S_i^z = (-1)^{(x_i + y_i + z_i)}$. However, such state is clearly is not even an eigenstate of the Heisenberg Hamiltonian since its $S_i^+ S_j^-$ terms interchange spins on sites i, j .

However, analogously to our analysis of an interacting superfluid (for which the strict BEC state is not a ground state), we can assume that this classical state is an approximate

ground state and then study corrections to it. In this approach we can again utilize the Holstein-Primakoff representation that we take to be distinct on the A and B sublattices,

$$\begin{aligned} S_{Ai}^+ &= (2S - a_i^\dagger a_i)^{1/2} a_i, \quad S_{Ai}^- = a_i^\dagger (2S - a_i^\dagger a_i)^{1/2}, \quad S_{Ai}^z = S - a_i^\dagger a_i, \text{ with } 0 \leq a_i^\dagger a_i \leq 2S, \\ S_{Bi}^+ &= b_i^\dagger (2S - b_i^\dagger b_i)^{1/2}, \quad S_{Bi}^- = (2S - b_i^\dagger b_i)^{1/2} b_i, \quad S_{Bi}^z = -S + b_i^\dagger b_i, \text{ with } 0 \leq b_i^\dagger b_i \leq 2S. \end{aligned} \quad (73)$$

Using this inside the Heisenberg Hamiltonian for the Néel state, we obtain a Bogoluibov-like Hamiltonian ($\mathbf{r}, \mathbf{r}'$ are nearest neighbors on a cubic lattice)

$$H_{AFM} \approx 2NzJS^2 - 2JS \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left(a_{\mathbf{r}}^\dagger a_{\mathbf{r}'} + b_{\mathbf{r}'}^\dagger b_{\mathbf{r}} + a_{\mathbf{r}} b_{\mathbf{r}'} + b_{\mathbf{r}'}^\dagger a_{\mathbf{r}}^\dagger \right), \quad (74)$$

that can be diagonalize via a Bogoluibov transformation

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} b_{-\mathbf{k}}^\dagger, \quad \beta_{\mathbf{k}} = u_{\mathbf{k}} b_{-\mathbf{k}} - v_{\mathbf{k}} a_{\mathbf{k}}^\dagger,$$

obtaining

$$H = E_0 + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left[\alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}} \right],$$

which on a cubic lattice gives:

$$E_0 = 2NzJS^2 + 2NzJS + \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}}, \quad (75)$$

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left((1 - \gamma_{\mathbf{k}}^2)^{-1/2} + 1 \right), \quad v_{\mathbf{k}}^2 = \frac{1}{2} \left((1 - \gamma_{\mathbf{k}}^2)^{-1/2} - 1 \right), \quad (76)$$

$$\hbar \omega_{\mathbf{k}} = 2|J|zS\sqrt{1 - \gamma_{\mathbf{k}}^2} \approx \left(2JS\sqrt{2za} \right) k, \quad (77)$$

where $\gamma_{\mathbf{k}} = \frac{1}{z} \sum_{\delta_j} e^{i\mathbf{k} \cdot \delta_j}$. Note that the Néel ground state is modified as the true ground state is annihilated by $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$, rather than by $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$.

As for an interacting superfluid, we can also compute the magnetization “depletion”, i.e., reduction in the staggered magnetization S by quantum fluctuations in the ground state. This is given by

$$\langle \delta S_z \rangle = \frac{2}{N} \sum_{\mathbf{k}} \langle AFM | a_{\mathbf{k}}^\dagger a_{\mathbf{k}} | AFM \rangle = \frac{1}{N} \sum_{\mathbf{k}} \left[(1 - \gamma_{\mathbf{k}}^2)^{-1/2} - 1 \right].$$

At finite T this is generalized to give

$$\langle \delta S_z \rangle = \frac{2}{N} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{e^{\beta \hbar \omega_{\mathbf{k}}} - 1} (1 - \gamma_{\mathbf{k}}^2)^{-1/2}.$$

With the spectrum at hand, AFM’s thermodynamics (susceptibility, heat capacity, etc) can be straightforwardly computed following standard analysis as for example done above for the FM state.

G. Spin-coherent states and Berry phase

An alternative and often very convenient description of magnetic states is in terms of spin coherent states (in analogy with coherent-state path-integral description of bosons). A coherent state

$$|\hat{\mathbf{n}}\rangle = U_{\hat{\mathbf{n}}}|S_z = S, \hat{\mathbf{z}}\rangle,$$

labeled by a unit vector $\hat{\mathbf{n}}$ is a highest-weight, $|S_z = S\rangle$ maximally polarized along the quantization axis $\hat{\mathbf{n}}$, satisfying

$$\hat{\mathbf{n}} \cdot \mathbf{S}|\hat{\mathbf{n}}\rangle = S|\hat{\mathbf{n}}\rangle.$$

$U_{\hat{\mathbf{n}}}$ is the SU(2) rotation, Eq. (59) of the $\hat{\mathbf{z}} \rightarrow \hat{\mathbf{n}}$, that can also be written as $U_{\hat{\mathbf{n}}} = e^{i\frac{\theta}{2}\hat{\mathbf{n}} \times \hat{\mathbf{z}} \cdot \boldsymbol{\sigma}}$. Spin coherent state can be expressed in terms of Schwinger bosons according to

$$|\hat{\mathbf{n}}\rangle = \frac{1}{\sqrt{2S!}}(ua^\dagger + vb^\dagger)^{2S}|0\rangle,$$

where the coherence factors form a coherent-state spinor

$$\begin{pmatrix} u \\ v \end{pmatrix} = e^{-i\chi/2} \begin{pmatrix} \cos \frac{1}{2}\theta \\ e^{+i\phi} \sin \frac{1}{2}\theta \end{pmatrix} \quad (78)$$

One can see that for spin-1/2

$$|\hat{\mathbf{n}}\rangle = u|\uparrow\rangle + v|\downarrow\rangle = \sum_{\alpha=\uparrow,\downarrow} z_\alpha |\alpha\rangle,$$

where spinor components given by

$$\langle \alpha | \hat{\mathbf{n}} \rangle \equiv \mathbf{z}_\alpha = \begin{pmatrix} u \\ v \end{pmatrix}_\alpha,$$

where $\alpha = \uparrow, \downarrow$, giving spinor representation $\hat{\mathbf{n}} = \mathbf{z}^\dagger \boldsymbol{\sigma} \mathbf{z}$, with $\mathbf{z}^\dagger \mathbf{z} = 1$. For spin-S, the coherent state can be written as a direct product of $2S$ *identical* spin-1/2 coherent states (to ensure it to be a highest weight state)

$$|\hat{\mathbf{n}}\rangle = |\mathbf{z}\rangle \otimes |\mathbf{z}\rangle \otimes \dots \otimes |\mathbf{z}\rangle.$$

The key relation for developing spin coherent-state path integral is the resolution of identity,

$$\hat{\mathbf{1}} = \frac{2S+1}{4\pi} \int d\hat{\mathbf{n}} |\hat{\mathbf{n}}\rangle \langle \hat{\mathbf{n}}|,$$

and coherent states overlap

$$\langle \hat{\mathbf{n}} | \hat{\mathbf{n}}' \rangle = (\bar{u}u' + \bar{v}v')^{2S} = (\mathbf{z}^\dagger \mathbf{z}')^{2S}, \quad (79)$$

$$= \frac{1}{2^S} (1 + \hat{\mathbf{n}} \cdot \hat{\mathbf{n}}')^S, \quad (80)$$

where we took advantage of the observation that $\langle \hat{\mathbf{z}} | \hat{\mathbf{n}}' \rangle = (u')^{2S} = [\cos^2(\theta/2)]^S = 1/2^S [1 + \cos \theta]^S = 1/2^S [1 + \hat{\mathbf{z}} \cdot \hat{\mathbf{n}}']^S$ and rotational invariance.

With these identities, we can now derive spin coherent-state path-integral as we did for a bosonic system. Using above resolution of identity, we deduce Trotter decomposition of the evolution operator over time $t = Nt/N = N\epsilon$,

$$\begin{aligned} \langle \hat{\mathbf{n}}(t) = \hat{\mathbf{n}}_N | e^{-i\hat{H}t/\hbar} | \hat{\mathbf{n}}(0) = \hat{\mathbf{n}}_0 \rangle &= \langle \hat{\mathbf{n}}_N | e^{-i\hat{H}\epsilon/\hbar} | \hat{\mathbf{n}}_{N-1} \rangle \langle \hat{\mathbf{n}}_{N-1} | e^{-i\hat{H}\epsilon/\hbar} | \hat{\mathbf{n}}_{N-1} \rangle \dots \\ &\quad \langle \hat{\mathbf{n}}_j | e^{-i\hat{H}\epsilon/\hbar} | \hat{\mathbf{n}}_{j-1} \rangle \dots \langle \hat{\mathbf{n}}_1 | e^{-i\hat{H}\epsilon/\hbar} | \hat{\mathbf{n}}_0 \rangle. \end{aligned} \quad (81)$$

The matrix elements can be evaluated for $\epsilon \ll 1$,

$$\langle \hat{\mathbf{n}}_j | e^{-i\hat{H}\epsilon/\hbar} | \hat{\mathbf{n}}_{j-1} \rangle = \langle \hat{\mathbf{n}}_j | \hat{\mathbf{n}}_{j-1} \rangle \left(1 - \frac{i\epsilon}{\hbar} \frac{\langle \hat{\mathbf{n}}_j | \hat{H} | \hat{\mathbf{n}}_{j-1} \rangle}{\langle \hat{\mathbf{n}}_j | \hat{\mathbf{n}}_{j-1} \rangle} + \dots \right), \quad (82)$$

$$\approx \langle \hat{\mathbf{n}}_j | \hat{\mathbf{n}}_{j-1} \rangle e^{-i\epsilon H[\hat{\mathbf{n}}_j, \hat{\mathbf{n}}_{j-1}]/\hbar}, \quad (83)$$

$$\approx \left(\mathbf{z}_j^\dagger \mathbf{z}_{j-1} \right)^{2S} e^{-i\epsilon H[\hat{\mathbf{n}}_j, \hat{\mathbf{n}}_{j-1}]/\hbar} = \left(1 - \mathbf{z}_j^\dagger (\mathbf{z}_j - \mathbf{z}_{j-1}) \right)^{2S} e^{-i\epsilon H[\hat{\mathbf{n}}_j, \hat{\mathbf{n}}_{j-1}]/\hbar}, \quad (84)$$

$$= e^{-2S\epsilon \mathbf{z}_j^\dagger \dot{\mathbf{z}}_j} e^{-i\epsilon H[\hat{\mathbf{n}}_j, \hat{\mathbf{n}}_{j-1}]/\hbar} \equiv e^{i d\mathcal{S}[\hat{\mathbf{n}}_j]/\hbar}, \quad (85)$$

where the action is given by

$$\mathcal{S}[\hat{\mathbf{n}}(t)] = \sum_{j=1}^{N-1} d\mathcal{S} = \int_0^t dt' [i2S\hbar \mathbf{z}^\dagger(t') \dot{\mathbf{z}}(t') - H[S\hat{\mathbf{n}}(t')]], \quad (86)$$

and the evolution operator is given by

$$\langle \hat{\mathbf{n}}(t) | e^{-i\hat{H}t/\hbar} | \hat{\mathbf{n}}(0) \rangle = \prod_{j=1}^{N-1} \left[\frac{2S+1}{4\pi} \int d\hat{\mathbf{n}}_j e^{i d\mathcal{S}[\hat{\mathbf{n}}_j]/\hbar} \right], \quad (87)$$

$$\equiv \int \mathcal{D}\hat{\mathbf{n}}(t) e^{i\mathcal{S}[\hat{\mathbf{n}}(t)]/\hbar} \quad (88)$$

where we took the continuum limit $N \rightarrow \infty$, ignored the higher order corrections that distinguish $\hat{\mathbf{n}}_j$ and $\hat{\mathbf{n}}_{j-1}$ inside $H[\hat{\mathbf{n}}_j, \hat{\mathbf{n}}_{j-1}]$, and dropped the boundary terms.

The first term in the action $\mathcal{S}[\hat{\mathbf{n}}(t)]$ is the Berry phase[10], $\mathcal{S}_B[\hat{\mathbf{n}}(t)]$, that arises from nontrivial overlap of coherent states, has the same structure as that of bosonic “ $p\dot{q}$ ” term,

and therefore gives a nontrivial action even for a vanishing Hamiltonian,

$$\mathcal{S}_B[\hat{\mathbf{n}}(t)] = -i\hbar \sum_{t'=0}^t \ln(\langle n(t') | n(t' - dt) \rangle) = -i\hbar \sum_{t'=0}^t \ln \{1 - \langle n(t') | [n(t') - |n(t' - dt)\rangle] \}, \quad (89)$$

$$= i\hbar \int_0^t dt' \langle \hat{\mathbf{n}}(t') | \partial_{t'} \hat{\mathbf{n}}(t') \rangle = i\hbar \int_0^t dt' \langle \hat{\mathbf{n}} | \nabla_{\hat{\mathbf{n}}} \hat{\mathbf{n}} \rangle \cdot \frac{d\hat{\mathbf{n}}}{dt'} = i\hbar \int \langle \hat{\mathbf{n}} | \nabla_{\hat{\mathbf{n}}} \hat{\mathbf{n}} \rangle \cdot d\hat{\mathbf{n}}, \quad (90)$$

$$\equiv \hbar S \int_0^t dt' \mathbf{A}_B(t') \cdot \frac{d\hat{\mathbf{n}}}{dt'} = \hbar S \oint \mathbf{A}_B \cdot d\hat{\mathbf{n}} = \hbar S \int \int (\nabla_{\hat{\mathbf{n}}} \times \mathbf{A}_B) \cdot (d\hat{\mathbf{n}} \times d\hat{\mathbf{n}}), \quad (91)$$

$$= i2S\hbar \int_0^t dt' \mathbf{z}^\dagger(t') \dot{\mathbf{z}}(t') = -\hbar S \int_0^t dt' (1 - \cos \theta) \dot{\phi} = -\hbar S \int (1 - \cos \theta(\phi)) d\phi, \quad (92)$$

$$= -\hbar S \int_{\phi(0)}^{\phi(t)} d\phi \int_0^{\theta(\phi)} d\theta' \sin \theta' \equiv -\hbar S \Omega. \quad (93)$$

In above we have chosen the global phase $\chi = 0$, defined Ω as the solid angle subtended by $\hat{\mathbf{z}}$, $\hat{\mathbf{n}}(0)$ and $\hat{\mathbf{n}}(t)$ and defined the Berry connection, $\mathbf{A}_B[\hat{\mathbf{n}}]$,

$$\mathbf{A}_B(\hat{\mathbf{n}}) = A_\phi \hat{\phi} = (1 - \cos \theta) \hat{\phi}, \quad (94)$$

with associated Berry flux density given by

$$\mathbf{B}_B(\hat{\mathbf{n}}) = \nabla_{\hat{\mathbf{n}}} \times \mathbf{A}_B(\hat{\mathbf{n}}) = \hat{\mathbf{n}}, \quad (95)$$

as can be seen from (91). In Cartesian coordinates, related to spherical via $\mathbf{A} \cdot d\hat{\mathbf{n}} = A_x dx + A_y dy + A_z dz = A_\phi d\phi + A_\theta d\theta + A_r dr$, we find

$$A_x = \frac{1}{2r} \frac{y}{z+r}, \quad A_y = -\frac{1}{2r} \frac{x}{z+r}, \quad A_z = 0.$$

Berry phase term $\mathcal{S}_B[\hat{\mathbf{n}}(t)]$ in the above coherent-state formulation is a crucial ingredient of capturing the dynamics of a spin, $\mathbf{S}$. As is clear from (91), it maps the dynamics of a spin (with $H = 0$) labelled by $\hat{\mathbf{n}}$ onto dynamics of a charge $\hbar S$, massless (since there is no $\frac{1}{2}(\dot{\hat{\mathbf{n}}})^2$ term) particle moving on a surface of a unit sphere ($|\hat{\mathbf{n}}| = 1$), with a magnetic monopole at its center producing magnetic field (95). Canonical formulation of quantum mechanics of a charged particle in a magnetic field exhibits spectrum of Landau levels (LL)[?], that at zero mass reduces to the lowest LL (LLL). The LLL degeneracy in flat space is given by the number of flux quanta through the surface, while on the sphere it is shifted by 1. Thus, the number of effective LLL degenerate states is given by

$$g = \frac{B \text{Area}}{\phi_0} + 1 = \frac{4\pi}{(2\pi\hbar/q)} + 1 = \frac{4\pi}{2\pi\hbar/(\hbar S)} + 1 = 2S + 1,$$

recovering the degeneracy of spin S and its correct partition function, $Z = 2S + 1$ for a vanishing Hamiltonian.

This Berry (also known as geometric, topological, or Wess-Zumino) phase term has a number of important properties. In particular[1, 9]

$$\delta\Omega[\hat{\mathbf{n}}(t)] = \int dt \left[\frac{\partial A_\beta}{\partial n_\alpha} \frac{dn_\beta}{dt} \delta n_\alpha + A_\alpha \frac{d}{dt} \delta n_\alpha \right], \quad (96)$$

$$= \int dt \left[\frac{\partial A_\beta}{\partial n_\alpha} - \frac{\partial A_\alpha}{\partial n_\beta} \right] \frac{dn_\beta}{dt} \delta n_\alpha = \int dt \delta \hat{\mathbf{n}} \cdot \left(\frac{d\hat{\mathbf{n}}}{dt} \times \hat{\mathbf{n}} \right), \quad (97)$$

which gives the expected precessional equation of motion for the spin labelled by $\hat{\mathbf{n}}(t)$

$$-\frac{\delta\mathcal{S}[\hat{\mathbf{n}}(t)]}{\delta\hat{\mathbf{n}}(t)} = \hbar S \frac{\delta\Omega[\hat{\mathbf{n}}(t)]}{\delta\hat{\mathbf{n}}(t)} + \frac{\partial H}{\partial \hat{\mathbf{n}}} = 0, \quad (98)$$

$$= \hbar S \frac{d\hat{\mathbf{n}}(t)}{dt} \times \hat{\mathbf{n}} + \frac{\partial H}{\partial \hat{\mathbf{n}}} = 0, \quad (99)$$

i.e., consistent with (38), we find

$$\hbar S \frac{\partial \hat{\mathbf{n}}(t)}{\partial t} = \frac{\partial H}{\partial \hat{\mathbf{n}}} \times \hat{\mathbf{n}},$$

in a effective magnetic field given by $\frac{\partial H}{\partial \hat{\mathbf{n}}}$. We note that above the projection transverse to $\hat{\mathbf{n}}$ is implicit, implemented by a Lagrange multiplier term $\int dt \lambda (\hat{\mathbf{n}}^2 - 1)$ added to the action.

Thus, $S_B[\hat{\mathbf{n}}(t)]$ is absolutely crucial for getting the correct spin dynamics even at the classical level. It is also essential for quantization of spin S as half-integers. To see the latter we note (in close analogy of Dirac's argument for quantization of electrical charge in inverse units of magnetic monopole charge), that for single-valueness of the evolution operator, $S_B/\hbar$ needs to be periodic modulo 2π , i.e., $\Omega = 4\pi$ must correspond to $S_B/\hbar = 2\pi n$, which requires $S = n/2$, $n \in \mathbb{Z}$.

Examining the expression for $\delta\Omega[\hat{\mathbf{n}}(t)]$, (97), we note that $\Omega[\hat{\mathbf{n}}(t)]$ may be expressible in a more covariant form, i.e., in terms of coherent-state label $\hat{\mathbf{n}}(t, s)$ extended along another "time" variable s , with $\hat{\mathbf{n}}(t, s = 1) \equiv \hat{\mathbf{n}}(t)$, $\hat{\mathbf{n}}(t, 0) \equiv \hat{\mathbf{z}}$,

$$\Omega[\hat{\mathbf{n}}(t)] = \int \delta\Omega[\hat{\mathbf{n}}(t)] = \int_0^1 ds \frac{d\Omega[\hat{\mathbf{n}}(t, s)]}{ds}, \quad (100)$$

$$= \int_0^1 ds \int dt \frac{\partial \hat{\mathbf{n}}(t, s)}{\partial s} \cdot \frac{\delta\Omega[\hat{\mathbf{n}}(t, s)]}{\delta \hat{\mathbf{n}}(t, s)}, \quad (101)$$

$$= \int_0^1 ds \int dt \hat{\mathbf{n}}(t, s) \cdot \left(\frac{\partial \hat{\mathbf{n}}}{\partial s} \times \frac{\partial \hat{\mathbf{n}}}{\partial t} \right) = \frac{1}{2} \int_0^1 \int d^2t \epsilon_{0jk} \hat{\mathbf{n}} \cdot (\partial_j \hat{\mathbf{n}} \times \partial_k \hat{\mathbf{n}}), \quad (102)$$

a form that for topologically stable configurations that wrap around the sphere gives an integer multiple of 4π and is referred to as the Pontryagin index. It is a Jacobian of the $S^2 \rightarrow S^2$, π_2 -mapping, associated with $\hat{\mathbf{n}}(s, t)$ wrapping around the sphere defined by (s, t) (with points at infinity identified).

1. Ferromagnetic excitations

expand about polarized phase in small fluctuations, compute Berry's vector potential and obtain action for small excitations including external magnetic field to show gap and its disappearance.

2. Antiferromagnetic excitations

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