Contents

7 QUANTUM MAGNETISM

The main purpose of this section is to introduce you to ordered magnetic states in solids and their "spin wave-like" elementary excitations. Magnetism is an enormous field, and reviewing it is beyond the scope of this course. I will for the most part assume you have been exposed to some of the basics before, but if not, they are extensively reviewed at an elementary level in Ashcroft & Mermin, and at a more advanced one by Mattis[1], and by White[2]. I will also lecture for a short time on the basics to refresh your memory a bit. What the classic texts cited above do not do is expose you to recent developments and current excitement in the field of low-dimensional magnetism, to which the last subsection here should serve as a portal.

7.1 Introduction

7.1.1 Atomic magnetic Hamiltonian

The simplest magnetic systems to consider are insulators where electron-electron interactions are weak. If this is the case, the magnetic response of the solid to an applied field is given by the sum of the susceptibilities of the individual atoms. The magnetic susceptibility is defined by the the 2nd derivative of the free energy,[3]

$$\chi = -\frac{\partial^2 F}{\partial H^2}. \tag{1}$$

We would like to know if one can understand (on the basis of an understanding of atomic structure) why some systems (e.g. some elements which are insulators) are paramagnetic ($\chi > 0$) and some diamagnetic ($\chi < 0$).

[1] D. Mattis, Theory of Magnetism I & II, Springer 1981
[2] R. White, Quantum Theory of Magnetism, McGraw-Hill, 1970
[3] In this section I choose units such that the system volume V = 1.

The one-body Hamiltonian for the motion of the electrons in the nuclear Coulomb potential in the presence of the field is

$$H_{atom} = \frac{1}{2m}\sum_i \left(\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i)\right)^2 + \sum_i V(r_i) + g_0\mu_B \mathbf{H}\cdot\mathbf{S}, \tag{2}$$

where $\Sigma_i \mathbf{S}_i$ is the total spin operator, $\mu_B \equiv e/(2mc)$ is the Bohr magneton, $g_0 \simeq 2$ is the gyromagnetic ratio, and $\mathbf{A} = -\frac{1}{2}\mathbf{r}\times\mathbf{H}$ is the vector potential corresponding to the applied uniform field, assumed to point in the $\hat{z}$ direction. Expanding the kinetic energy, H_{atom} may now be expressed in terms of the orbital magnetic moment operator $\mathbf{L} = \Sigma_i \mathbf{r}\times\mathbf{p}_i$ as

$$\begin{aligned} H_{atom} &= \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_i V(r_i) + \delta H, && (3)\\ \delta H &= \mu_B(\mathbf{L} + g_0\mathbf{S})\cdot\mathbf{H} + \frac{e^2}{8mc^2}H^2\sum_i(x_i^2 + y_i^2). && (4)\end{aligned}$$

Given a set of exact eigenstates for the atomic Hamiltonian in zero field $|n\rangle$ (ignore degeneracies for simplicity), standard perturbation theory in δH gives

$$\delta E_n = \mathbf{H}\cdot\langle n|\vec{\mu}|n\rangle + \sum_{n\neq n'} |\frac{\langle n|\mathbf{H}\cdot\vec{\mu}|n'\rangle|^2}{E_n - E_{n'}} + \frac{e^2}{8mc^2}H^2\langle n|\sum_i(x_i^2+y_i^2)|n\rangle, \tag{5}$$

where $\vec{\mu} = \mu_B(\mathbf{L}+g_0\mathbf{S})$. It is easy to see that the first term dominates and is of order the cyclotron frequency $\omega_c \equiv eH/(mc)$ unless it vanishes for symmetry reasons. The third term is of order $\omega_c/(e^2/a_0)$ smaller, because typical electron orbits are confined to atomic sizes a_0, and is important in insulators only when the state $|n\rangle$ has zero magnetic moment ($L = S = 0$). Since the coefficient of H^2 is manifestly positive, the susceptibility[4] in the $\mu = 0$ ground state $|0\rangle$ is $\chi = -\partial^2\delta E_0/\partial H^2$, which is clearly < 0, i.e. diamagnetic.[5]

[4] If the ground state is nondegenerate, we can replace $F = E - TS$ in the definition of the susceptibility by the ground state energy E_0.

[5] This weak diamagnetism in insulators with filled shells is called Larmor diamagnetism

In most cases, however, the atomic shells are partially filled, and the ground state is determined by minimizing the atomic energy together with the intraatomic Coulomb interaction needed to break certain degeneracies, i.e. by "Hund's rules".[6] Once this ground state (in particlular the S, L, and J quantum numbers is known, the atomic susceptibility can be calculated. The simplest case is again the $J = 0$ case, where the first term in (5) again vanishes. Then the second term and third term compete, and can result in either a diamagnetic or paramagnetic susceptibility. The 2nd term is called the *Van Vleck* term in the energy. It is paramagnetic since its contribution to χ is

$$\chi_{VV} = -\frac{\partial^2 E_0|_{2nd\ term}}{\partial H^2} = 2\mu_B^2 \sum_n \frac{|\langle 0|\vec{\mu}|n'\rangle|^2}{E_n - E_0} > 0. \tag{6}$$

7.1.2 Curie Law-free spins

In the more usual case of $J \neq 0$, the ground state is $2J+1$ degenerate, and we have to be more careful about defining the susceptibility. The free energy as $T \to 0$ can no longer be replaced by E_0 as we did above. We have to account for the entropy of the $2J+1$ degenerate spin states as well. Applying a magnetic field breaks this degeneracy, so we have a small statistical calculation to do. The energies of the "spin" in a field are given by

$$H = -\vec{\mu} \cdot \mathbf{H}, \tag{7}$$

and since $\vec{\mu} = -\gamma \mathbf{J}$ within the subspace of definite J^2,[7] the $2J+1$ degeneracy in H = 0 is completely broken. The free energy is

$$F = -T \log Z \ = \ -T \log \sum_{J_z=-J}^{J} e^{\beta\gamma H J_z}$$

[6] see any serious quantum mechanics book

[7] This is not obvious at first sight. The magnetic moment *operator* $\vec{\mu} \propto \hat{\mathbf{L}} + \mathbf{g_0}\hat{\mathbf{S}}$ is not proportional to the total angular momentum *operator* $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$. However its matrix elements *within the subspace of definite* L, S, J are proportional, due to the Wigner-Eckart theorem. One therefore may assume the proportionality within the subspace, where the proportionality const. $\gamma = g(J, L, S)\mu_B$. g is called Landé g-factor, and is independent of J_z according to Wigner-Eckart. See e.g. Ashcroft & Mermin p. 654.

$$= -T \log \left[\frac{e^{\beta\gamma H(J+1/2)} - e^{-\beta\gamma H(J+1/2)}}{e^{\beta\gamma H/2} - e^{-\beta\gamma H/2}} \right], \tag{8}$$

so the magnetization of the free spins is

$$M = -\frac{\partial F}{\partial H} = \gamma J B(\beta\gamma J H), \tag{9}$$

where $B(x)$ is the Brillouin function

$$B(x) = \frac{2J+1}{2J} \coth \frac{2J+1}{2J} x - \frac{1}{2J} \coth \frac{1}{2J} x. \tag{10}$$

Note I defined $\gamma = \mu_B g$. We were particularly interested in the $H \to 0$ case, so as to compare with ions with filled shells or $J = 0$; in this case one expands for $T >> \gamma H$, i.e. $\coth x \sim 1/x + x/3 + \ldots$, $B(x) \simeq (J+1)x/(3J)$ to find the susceptibility

$$\boxed{\chi = -\frac{\partial^2 F}{\partial H^2} = \frac{\gamma^2 J(J+1)}{3T}}, \tag{11}$$

i.e. a *Curie law* for the high-temperature susceptibility. A $1/T$ susceptibility at high T is generally taken as evidence for free paramagnetic spins, and the size of the moment given by $\mu^2 = \gamma^2 J(J+1)$.

7.1.3 Magnetic interactions

The most important interactions between magnetic moments in an insulator are electrostatic and inherently quantum mechanical in nature. From a classical perspective, one might expect two such moments to interact via the classical dipolar force, giving a potential energy of configuration of two moments $\vec{\mu}_1$ and $\vec{\mu}_2$ separated by a distance $\mathbf{r}$ of

$$U = \frac{\vec{\mu}_1 \cdot \vec{\mu}_2 - 3(\vec{\mu}_1 \cdot \hat{r})(\vec{\mu}_1 \cdot \hat{r})}{r^3} \tag{12}$$

Putting in typical atomic moments of order $\mu_B = e\hbar/mc$ and distances of order a Bohr radius $r \sim a_0 = \hbar^2/me^2$, we find $U \simeq 10^{-4} eV$, which is very small compared to typical atomic energies of order eV. Quantum-mechanical *exchange* is almost aways a much larger effect, and the dipolar interactions are therefore normally neglected in the discussions of magnetic interactions in solids. Exchange arises because, e.g., two quantum mechanical spins 1/2 (in isolation) can be in either a spin triplet (total $S = 1$), or singlet (total $S = 0$). The spatial part of the two-particle wavefunctions is antisymmetric for triplet and symmetric for singlet, respectively. Since the particles carrying the spins are also charged, there will be a large energetic difference between the two spin configurations due to the different size of the Coulomb matrix elements (the "amount of time the two particles spend close to each other") in the two cases.[8] In terms of hypothetical atomic wave functions $\psi_a(\mathbf{r})$ and $\psi_b(\mathbf{r})$ for the two particles, the singlet and triplet combinations are $\psi_{\substack{0\\1}}(\mathbf{r}_1, \mathbf{r}_2) = \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) \pm \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)$, so the singlet-triplet splitting is approximately

$$\begin{aligned} -J \equiv E_0 - E_1 &= \langle 0|H|0\rangle - \langle 1|H|1\rangle \\ &\simeq 2\int d^3r_1 d^3r_2 \psi_a^*(\mathbf{r}_1)\psi_b^*(\mathbf{r}_2) V(\mathbf{r}_1, \mathbf{r}_2)\psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1), \end{aligned} \tag{13}$$

where V represents the Coulomb interactions between the particles (and possible other particles in the problem).[9]

We'd now like to write down a simple Hamiltonian for the spins which contains the physics of this exchange splitting. This was done first by Heisenberg (check history here), who suggested

$$H_{2-spin} = J\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 \tag{15}$$

[8]Imagine moving 2 H-atoms together starting from infinite separation. Initially the 3 $S = 1$ states and 1 $S = 0$ states must be degenerate. As the particles start to interact via the Coulomb force at very long range, there will be a splitting between singlet and triplet.

[9]For example, in the H molecule,

$$V(\mathbf{r}_1, \mathbf{r}_2) = \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + \frac{e^2}{|\mathbf{R}_1 - \mathbf{R}_2|} - \frac{e^2}{|\mathbf{r}_1 - \mathbf{R}_1|} - \frac{e^2}{|\mathbf{r}_2 - \mathbf{R}_2|}, \tag{14}$$

where $\mathbf{R}_1$ and $\mathbf{R}_2$ are the sites of the protons. Note the argument above would suggest naively that the triplet state should be the ground state in the well-separated ion limit, because the Coulomb interaction is minimized in the spatially antisymmetric case. However the true ground state of the H_2 molecule is the Heitler-London *singlet* state $\psi_s(\mathbf{r}_1, \mathbf{r}_2) \simeq \psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)$

You can easily calculate that the energy of the triplet state in this Hamiltonian is $J/4$, and that of the singlet state $-3J/4$. So the splitting is indeed J. Note that the sign of J in the H_2 case is positive, meaning the $S = 0$ state is favored; the interaction is then said to be antiferromagnetic, meaning it favors antialigning the spins with each other.[10]

The so-called Heitler-London model of exchange just reviewed presented works reasonably well for well-separated molecules, but for N atoms in a real solid, magnetic interactions are much more complicated, and it is in general not sufficient to restrict one's consideration to the 4-state subspace (singlet $\oplus$ 3 components of triplet) to calculate the effective exchange. In many cases, particularly when the magnetic ions are reasonably well-separated, it nevertheless turns out to be ok to simply extend the 2-spin form (15) to the entire lattice:

$$H = J \sum_{i\delta} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\delta} \tag{16}$$

where J is the exchange constant, i runs over sites and δ runs over nearest neighbors.[11] This is the so-called Heisenberg model. The sign of J can be either antiferromagnetic ($J > 0$ in this convention), or ferromagnetic ($J < 0$). This may lead, at sufficiently low temperature, to a quantum ordered state with ferromagnetic or antiferromagnetic-type order. Or, it may not. A good deal depends on the type and dimensionality of the lattice, as we discuss below.

Although oversimplified, the Heisenberg model is still very difficult to solve. Fortunately, a good deal has been learned about it, and once one has put in the work it turns out to describe magnetic ordering and magnetic correlations rather well for a wide class of solids, provided one is willing to treat J as a phenomenological parameter to be determined from a fit

[10] Historically the sign convention for J was the opposite; $J > 0$ was usually taken to be ferromagnetic, i.e. the Hamiltonian was defined with another minus sign. I use the more popular convention $H = J \sum S_i \cdot S_j$. Be careful!

[11] One has to be a bit careful about the counting. J is defined conventionally such that there is one term in the Hamiltonian for each *bond* between two sites. Therefore if i runs over all sites, one should have δ only run over, e.g. for the simple cubic lattice, $+\hat{x}$, $+\hat{y}$, and $+\hat{z}$. If it ran over all nearest neighbors, bonds would be double-counted and we would have to multiply by $1/2$.

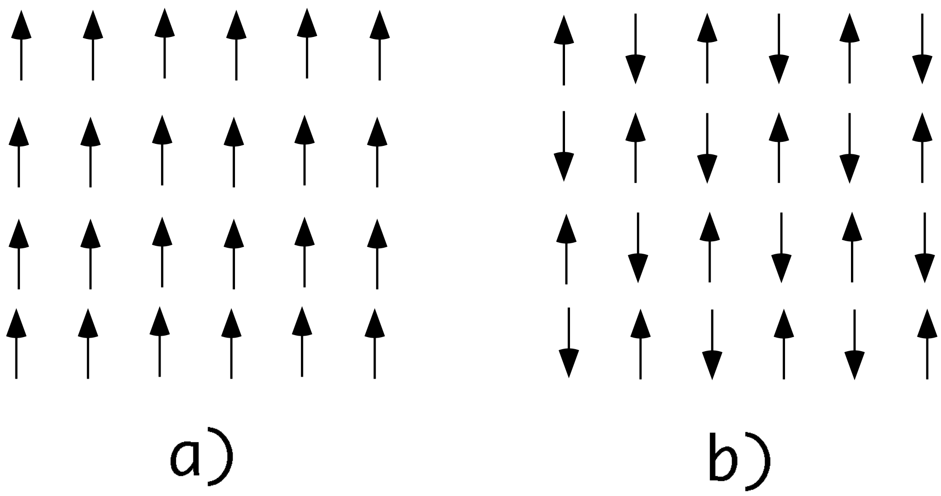


Figure 1: a) Ferromagnetic ordering; b) antiferromagnetic ordering.

to experiment.

The simplest thing one can do to take interactions between spins into account is to ask, "What is the average exchange felt by a given spin due to all the other spins?" This is the essence of the *molecular field theory* or *mean field theory* due to Weiss. Split off from the Hamiltonian all terms connecting any spins to a specific spin $\hat{\mathbf{S}}_i$. For the nearest-neighbor exchange model we are considering, this means just look at the nearest neighbors. This part of the Hamiltonian is

$$\delta H_i = \hat{\mathbf{S}}_i \cdot \left[J \sum_\delta \hat{\mathbf{S}}_{i+\delta} \right] - \vec{\mu} \cdot \mathbf{H}, \tag{17}$$

where we have included the coupling of the spin in question to the external field as well. We see that the 1-spin Hamiltonian looks like the Hamiltonian for a spin in an effective field,

$$\delta H_i = -\vec{\mu}_i \cdot \mathbf{H}_{eff}, \tag{18}$$

$$\mathbf{H}_{eff} = \mathbf{H} - \frac{J}{g\mu_B} \sum_\delta \hat{\mathbf{S}}_{i+\delta} \tag{19}$$

Note this "effective field" as currently defined is a complicated *operator*, depending on the neighboring spin operators $\hat{\mathbf{S}}_{i+\delta}$. The mean field theory replaces this quantity with its thermal average

$$\mathbf{H}_{eff} = \mathbf{H} - \frac{J}{g\mu_B}\sum_\delta \langle \hat{\mathbf{S}}_{i+\delta}\rangle \tag{20}$$

$$= \mathbf{H} - \frac{zJ}{(g\mu_B)^2}\mathbf{M}, \tag{21}$$

where the magnetization $M = \langle \mu \rangle$ and z is the number of nearest neighbors again. But since we have an effective one-body Hamiltonian, thermal averages are supposed to be computed just as in the noninteracting system, cf. (9), but in the ensemble with effective magnetic field. Therefore the magnetization is

$$M = \gamma S B(\beta\gamma S H_{eff}) = \gamma S B\left(\beta\gamma S[H - \frac{zJ}{\gamma^2}M]\right). \tag{22}$$

This is now a nonlinear equation for M, which we can solve for any H and T. It should describe a ferromagnet with finite spontaneous ($H \to 0$) magnetization below a critical temperature T_c. So to search for T_c, set $H = 0$ and expand $B(x)$ for small x:

$$M = -\gamma S B\left(\frac{zJ}{\gamma T_c}M\right) \simeq -\gamma S\ \frac{S+1}{3S}\ \frac{zJ}{\gamma T_c}M \tag{23}$$

$$\Rightarrow\ T_c = \frac{S(S+1)}{3}z(-J), \tag{24}$$

So the critical temperature in this mean field theory (unlike the BCS mean field theory!) is of order the fundamental interaction energy $|J|$. We expect this value to be an upper bound to the true critical temperature, which will be supressed by spin fluctuations about the mean field used in the calculation.

Below T_c, we can calculate how the magnetization varies near the transition by expanding the Brillouin fctn. to one higher power in x. The result is (fill in)

$$M = xxx(T - T_c)^{1/2}. \tag{25}$$

Note this exponent 1/2 is characteristic of the disappearance of the order parameter near the transition of any mean field theory (Landau).

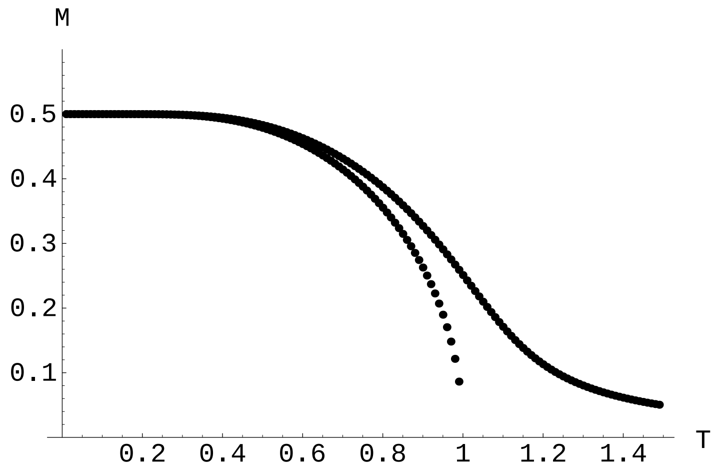


Figure 2: Plot of Mathematica solution to eqn. (22) for M vs. T using $-J = g = 1$; $z = 4$; $S = 1/2$. T_c=1 for this choice. Upper curve: $H = 0.1$; lower curve: $H = 0$.

7.2 Ferromagnetic magnons

Let's consider the simplest example of an insulating ferromagnet, described by the ferromagnetic Heisenberg Hamiltonian

$$H = J \sum_{i\delta} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+\delta} - 2\mu_B H_0 \sum_i \hat{S}_{iz}, \tag{26}$$

where $J < 0$ is the ferromagnetic exchange constant, i runs over sites and δ runs over nearest neighbors, and H_0 is the magnetic field pointing in the $\hat{z}$ direction. It is clear that the system can minimize its energy by having all the spins $\mathbf{S}$ align along the $\hat{z}$ direction at $T = 0$; i.e. the quantum ground state is identical to the classical ground state. Finding the elementary excitations of the quantum many-body system is not so easy, however, due to the fact that the spin operators do not commute.

7.2.1 Holstein-Primakoff transformation

One can attempt to transform the spin problem to a more standard many-body interacting problem by replacing the spins with boson creation and annihilation operators. This can be done *exactly* by the Holstein-Primakoff transformation[12]

$$\hat{S}_i^+ = \hat{S}_{ix} + i\hat{S}_{iy} = (2S)^{1/2}\left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2} a_i \tag{27}$$

$$\hat{S}_i^- = \hat{S}_{ix} - i\hat{S}_{iy} = (2S)^{1/2} a_i^\dagger \left(1 - \frac{a_i^\dagger a_i}{2S}\right)^{1/2}. \tag{28}$$

Verify for yourselves that these definitions $S_i^\pm$ give the correct commutation relations $[\hat{S}_x, \hat{S}_y] = i\hat{S}_z$ *if* the bosonic commutation relations $[a, a^\dagger] = 1$ are obeyed on a given lattice site. Note also that the operators which commute with the Hamiltonian are $\hat{S}^2$ and $\hat{S}_z$ as usual, so we can classify all states in terms of their eigenvalues $S(S+1)$ and S_z. To complete the algebra we need a representation for $\hat{S}_z$, which can be obtained by using the identity (on a given site i)

$$\hat{S}_z^2 = S(S+1) - \frac{1}{2}\left(\hat{S}^+\hat{S}^- + \hat{S}^-\hat{S}^+\right). \tag{29}$$

Using (28) and some tedious applications of the bosonic commutation relations, we find

$$\hat{S}_z = S - a^\dagger a. \tag{30}$$

Now since the system is periodic, we are looking for excitations which can be characterized by a well-defined momentum (crystal momentum) $\mathbf{k}$, so we define the Fourier transformed variables

$$a_i = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{x}_i}\, b_{\mathbf{k}} \quad ; a_i^\dagger = \frac{1}{N^{1/2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}_i}\, b_{\mathbf{k}}^\dagger, \tag{31}$$

where as usual the F.T. variables also satisfy the bosonic relations $[b_{\mathbf{k}}, b_{\mathbf{k}'}] = \delta_{\mathbf{k}\mathbf{k}'}$, etc. Looking forward a bit, we will see that the operators $b_{\mathbf{k}}^\dagger$ and $b_{\mathbf{k}}$

[12] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

create and destroy a *magnon* or *spin-wave* excitation of the ferromagnet. These turn out to be excitations where the spins locally deviate only a small amount from their ground state values ($\parallel \hat{z}$) as the "spin wave" passes by. This suggests *a posteriori* that an expansion in the spin *deviations* $a_i^\dagger a_i$ (see (30)) may converge quickly. Holstein and Primakoff therefore suggested expanding the nasty square roots in (28), giving

$$
\begin{aligned}
\hat{S}_i^+ &\simeq (2S)^{1/2}\left[a_i - \left(\frac{a_i^\dagger a_i a_i}{4S}\right) + \ldots\right] \\
&= \left(\frac{2S}{N}\right)^{1/2}\left[\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} b_{\mathbf{k}} - \frac{1}{4SN}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} e^{i(\mathbf{k}-\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} b_{\mathbf{k}''} + \ldots\right], \qquad (32) \\
\hat{S}_i^- &\simeq (2S)^{1/2}\left[a_i^\dagger - \left(\frac{a_i^\dagger a_i^\dagger a_i}{4S}\right) + \ldots\right] \\
&= \left(\frac{2S}{N}\right)^{1/2}\left[\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger - \frac{1}{4SN}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} e^{i(\mathbf{k}+\mathbf{k}'-\mathbf{k}'')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}^\dagger b_{\mathbf{k}''} + \ldots\right], \qquad (33) \\
\hat{S}_{iz} &= S - a_i^\dagger a_i = S - \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'}. \qquad (34)
\end{aligned}
$$

Note that the expansion is formally an expansion in $1/S$, so we might expect it to converge rapidly in the case of a large-spin system.[13] The last equation is exact, not approximate, and it is useful to note that the total spin of the system along the magnetic field is

$$S_{z,tot} = \sum_i S_z = NS - \frac{1}{N}\sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \qquad (35)$$

consistent with our picture of magnons tipping the spin away from its $T = 0$ equilibrium direction along the applied field.

[13]For spin-1/2, the case of greatest interest, however, it is far from obvious that this uncontrolled approximation makes any sense, despite the words we have said about spin deviations being small. Why should they be? Yet empirically linear spin wave theory works very well in 3D, and surprisingly well in 2D.

7.2.2 Linear spin wave theory

The idea now is to keep initially only the bilinear terms in the magnon operators, leaving us with a soluble Hamiltonian, hoping that we can then treat the 4th-order and higher terms perturbatively.[14] Simply substitute (32)-(34) into (26), and collect the terms first proportional to S^2, S, 1, $1/S$, etc. We find

$$H = \frac{1}{2} JNzS^2 - 2\mu_B H_0 S + H_0^{magnon} + \mathcal{O}(1), \tag{36}$$

where z is the number of nearest neighbors (e.g. 6 for simple cubic lattice), and

$$\begin{aligned} H_0^{magnon} &= \frac{JS}{N} \sum_{i\delta\mathbf{k}\mathbf{k}'} \Big[e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{i\mathbf{k}\cdot\delta} b_{\mathbf{k}} b_{\mathbf{k}'}^\dagger + e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{-i\mathbf{k}\cdot\delta} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \\ &\quad - e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} e^{i\mathbf{k}\cdot\delta} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} - e^{-i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{R}_i+\delta)} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \Big] + \frac{2\mu_B H_0}{N} \sum_{i\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger b_{\mathbf{k}'} \\ &= JzS \sum_{\mathbf{k}} \Big[\gamma_{\mathbf{k}} b_{\mathbf{k}} b_{\mathbf{k}}^\dagger + \gamma_{-\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} - 2 b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \Big] + 2\mu_B H_0 \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \\ &= \sum_{\mathbf{k}} \left[-2JzS(1-\gamma_{\mathbf{k}}) + 2\mu_B H_0 \right] b_{\mathbf{k}}^\dagger b_{\mathbf{k}}, \end{aligned} \tag{37}$$

where

$$\gamma_k = \frac{1}{z} \sum_{\delta} e^{i\mathbf{k}\cdot\delta} \tag{38}$$

is the magnon dispersion function, which in this approximation depends only on the positions of the nearest neighbor spins. Note in the last step of (37), I assumed $\gamma_{\mathbf{k}} = \gamma_{-\mathbf{k}}$, which is true for lattices with inversion symmetry. For example, for the simple cubic lattice in 3D with lattice constant a, $\gamma_{\mathbf{k}} = (\cos k_x a + \cos k_y a + \cos k_z a)/3$, clearly an even function of $\mathbf{k}$. Under these assumptions, the magnon part of the Hamiltonian is remarkably simple, and can be written like a harmonic oscillator or phonon-type Hamiltonian, $H_0^{magnon} = \Sigma_{\mathbf{k}}\, n_{\mathbf{k}} \omega_{\mathbf{k}}$, where $n_{\mathbf{k}} = b_{\mathbf{k}}^\dagger b_{\mathbf{k}}$ is the number of magnons in state $\mathbf{k}$, and

$$\omega_k = -JSz(1-\gamma_{\mathbf{k}}) + 2\mu_B H_0 \tag{39}$$

[14] physically these "nonlinear spin wave" terms represent the interactions of magnons, and resemble closely terms representing interactions of phonons in anharmonic lattice theory

is the magnon dispersion. The most important magnons will be those with momenta close to the center of the Brillouin zone, $k \sim 0$, so we need to examine the small-k dispersion function. For a Bravais lattice, like simple cubic, this expansion gives $1 - \gamma_{\mathbf{k}} \simeq k^2$,[15] i.e. the magnon dispersion vanishes as $k \to 0$. For more complicated lattices, there will be solutions with $\omega_{\mathbf{k}} \to$ const. There is always a "gapless mode" $\omega_{\mathbf{k}} \to 0$ as well, however, since the existence of such a mode is guaranteed by the Goldstone theorem.[16] The figure shows a simple 1D schematic of a spin

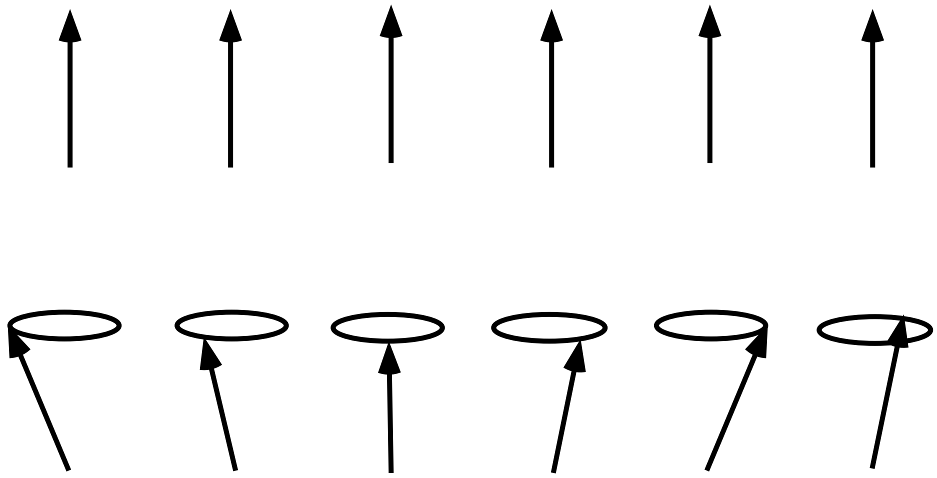


Figure 3: Real space picture of spin deviations in magnon. Top: ordered ground state

wave with wavelength $\lambda = 2\pi/k$ corresponding to about 10 lattice sites. The picture is supposed to convey the fact that the spin deviations from the ordered state are small, and vary slightly from site to site. Quantum mechanically, the wave function for the spin wave state contains at each site a small amplitude for the spin to be in a state with definite S_x and/or S_y. This can be seen by inverting Eq. (33) to leading order, & noting that the spin wave creation operator $b_{\mathbf{k}}^\dagger$ lowers the spin with $\hat{\mathbf{S}}^- = \hat{S}_x - i\hat{S}_y$ with phase $e^{-i\mathbf{k}\cdot\mathbf{R}_i}$ and amplitude $\sim 1/S$ at each site i.

[15] Check for simple cubic!

[16] For every spontaneously broken continuous symmetry of the Hamiltonian there is a $\omega_{\mathbf{k}\to 0} = 0$ mode.

7.2.3 Dynamical Susceptibility

Experimental interlude

The simple spin wave calculations described above (and below) are uncontrolled for spin-1/2 systems, and it would be nice to know to what extent one can trust them. In recent years, numerical work (exact diagonalization and quantum Monte Carlo) techniques have shown, as noted, that linear spin wave calculations compare suprisingly well with such "exact" results for the Heisenberg model. But we still need to know if there are any physical systems whose effective spin Hamiltonian can really be described by Heisenberg models. In addition, keep in mind that the utility of spin wave theory was recognized long before such numerical calculations were available, mainly through comparison with experiments on simple magnets. The most useful probe of magnetic structure is slow neutron scattering, a technique developed in the 40's by Brockhouse and Schull (Nobel prize 1994). This section is a brief discussion of how one can use neutron scattering techniques to determine the dispersion and lifetimes of magnetic excitations in solids.[17]

Neutrons scatter from solids primarily due to the nuclear strong force, which leads to nonmagnetic neutron-ion scattering and allows structural determinations very similar to x-ray diffraction analysis. In addition, slow neutrons traversing a crystal can emit or absorb phonons, so the inelastic neutron cross-section is also a sensitive measure of the dispersion of the collective modes of the ionic system.[18] There is also a force on the neutron due to the interaction of its small magnetic dipole moment with the spin magnetic moment of the electrons in the solid. There are therefore additional contributions to the peaks in the elastic neutron scattering intensity (at the Bragg angles) corresponding to magnetic scattering if the solid has long-range magnetic order; they can be distinguished from the

[17] A complete discussion is found in Lovesey, *Theory of Neutron Scattering from Condensed Matter, Oxford 1984, V. 2*

[18] cf. Ashcroft & Mermin ch. 24

nonmagnetic scattering because the additional spectral weight is strongly temperature dependent and disappears above the critical temperature, or through application of an external magnetic field. Furthermore, in analogy to the phonon case, inelastic neutron scattering experiments on ferromagnets yield peaks corresponding to processes where the neutron absorbs or emits a spin wave excitation. Thus the dispersion relation for the magnons can be mapped out.[19]

I will not go through the derivation of the inelastic scattering cross section, which can be found in Lovesey's book. It is similar to the elementary derivation given by Ashcroft & Mermin in Appendix N for phonons. The result is

$$\begin{aligned}\left(\frac{d^2\sigma}{d\Omega d\omega'}\right)_{inel} &= a_0^2\frac{k'}{k}\left\{\frac{g}{2}F(\mathbf{q})\right\}^2 e^{-2W(\mathbf{q})}\left(1+b(\omega)\right) \\ &\quad\times\frac{-N}{\pi(g\mu_B)^2}\sum_{\alpha\beta}(\delta_{\alpha\beta}-\hat{q}_\alpha\hat{q}_\beta)\ \mathrm{Im}\ \chi_{\alpha\beta}(\mathbf{q},-\omega), \qquad (40)\end{aligned}$$

where a_0 is the Bohr radius, $\mathbf{k}$ and $\mathbf{k}'$ are initial and final wave vector, $\mathbf{q}=\mathbf{k}-\mathbf{k}'$, $F(\mathbf{q})$ atomic form factor, $e^{-2W(\mathbf{q})}$ the Debye-Waller factor, and $b(\omega)$ the Bose distribution function, N the number of unit cells, and ω is the energy change of the neuton, $k^2/(2m)-k'^2/(2m)$. The physics we are interested in is contained in the imaginary part of the dynamic susceptibility $\chi(\mathbf{q},\omega)$. For $\omega<0$, this measures the energy loss by neutrons as they slow down while emitting spin waves in the solid; for $\omega>0$ the neutrons are picking up energy from thermally excited spin waves.

By spin rotational invariance, all components $\chi_{zz}=\chi_{xx}=\chi_{yy}$ are equal. It is then most convenient to calculate—within linear spin wave theory—the transverse spin susceptibility

$$\chi^R_{+-}(\mathbf{R}_i-\mathbf{R}_j,t)\equiv -\mathrm{Tr}\left(\hat{\rho}[\hat{\mathbf{S}}_i^+(t),\hat{\mathbf{S}}_j^-]\right)\theta(t) \qquad (41)$$

[19]Even in systems without long range magnetic order, neutron experiments provide important information on the correlation length and lifetime of *spin fluctuations*. In strongly correlated systems (e.g. magnets just above their critical temperature, or itinerant magnets close to a magnetic transition as in Sec. xxx), these can be thought of as collective modes with finite lifetime and decay length. This means the correlation function $\langle\hat{\mathbf{S}}_i^\alpha(t)\hat{\mathbf{S}}_j^\alpha\rangle$ is not const. as $t,|\mathbf{R}_i-\mathbf{R}_j|\to\infty$, but may fall off very slowly, as "power laws" $t^{-\beta}$, $|\mathbf{R}_i-\mathbf{R}_j|^{-\gamma}$.

and then its Fourier transform wrt momentum $\mathbf{q}$ and frequency ω. To do this, we proceed as usual and first calculate the Matsubara time-ordered function

$$\chi_{+-}(\mathbf{R}_i - \mathbf{R}_j, \tau) = -\mathrm{Tr}\ \left(\hat{\rho}\ T_\tau\ \hat{\mathbf{S}}_i^+(\tau)\hat{\mathbf{S}}_j^-(0)\right) \tag{42}$$

and substituting the linear expressions for $\hat{\mathbf{S}}^+$ and $\hat{\mathbf{S}}^-$ from (32) and (33). Then

$$\begin{aligned}
\chi_{+-}(\mathbf{R}_i - \mathbf{R}_j, \tau) &\simeq -(2S)\mathrm{Tr}\ \left(\hat{\rho}_0\ T_\tau\ a_i(\tau)a_j^\dagger(0)\right) \\
&= -(\frac{2S}{N})\sum_{\mathbf{q}\mathbf{q}'} e^{-i(\mathbf{q}\cdot\mathbf{R}_i - \mathbf{q}'\cdot\mathbf{R}_j)}\mathrm{Tr}\ \left(\hat{\rho}_0\ T_\tau\ b_\mathbf{q}(\tau)b_{\mathbf{q}'}^\dagger\right) \\
&= -(\frac{2S}{N})\sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\mathrm{Tr}\ \left(\hat{\rho}_0\ T_\tau\ b_\mathbf{q}(\tau)b_{\mathbf{q}}^\dagger\right). \quad (43)
\end{aligned}$$

But in the linear spin wave approximation, the leading-order approximate density matrix ρ_0 is just $\exp(-\beta H_0^{magnon})$, where $H_0^{magnon} = \Sigma_q\, \omega_\mathbf{q} b_\mathbf{q}^\dagger b_\mathbf{q}$. The trace therefore just yields the free boson Green's function, whose form we know. The Fourier transform with respect to time τ and space $\mathbf{R}_i - \mathbf{R}_j$ therefore gives

$$\chi_{+-}(\mathbf{q}, \omega_n) = (\frac{2S}{N})\left(\frac{1}{i\omega_n - \omega_\mathbf{q}}\right) \tag{44}$$

and analytically continuing as usual to the real axis shows finally that

$$\chi_{+-}(\mathbf{q}, \omega) = (\frac{2S}{N})\left(\frac{1}{\omega - \omega_\mathbf{q} + i0^+}\right) \tag{45}$$

so the final cross section is proportional to

$$\mathrm{Im}\ \chi_{+-}(\mathbf{q}, -\omega) \sim \delta(\omega + \omega_\mathbf{q}), \tag{46}$$

i.e. there is a peak when a magnon is *absorbed* (neutron's energy $k'^2/(2m)$ is larger than initial energy $k^2/(2m) \Rightarrow \omega \equiv k^2/(2m) - k'^2/(2m) < 0.$). There is another similar contribution proportional to $\delta(\omega - \omega_\mathbf{q})$ (emission) coming from χ_{-+}. Thus the dispersion $\omega_\mathbf{q}$ can be mapped out by careful measurement.

Figure 4: Neutron scattering data on ferromagnet

The one-magnon lines are of course broadened by magnon-magnon interactions, and by finite temperatures (Debye-Waller factor). There are also multimagnon absorption and emission processes which contribute in higher order.

7.2.4 Continuum description

In this section I will derive the continuum theory of spin wave excitations in a ferromagnet, useful when one is interested in long-wavelength properties. The microscopic details are integrated out, leaving an effective free energy which depends only on the magnetization *density* $M(\mathbf{r})$. The exchange energy per unit volume turns out to be

$$\mathcal{H} = \frac{1}{2}\rho_{s0} \sum_{\mu,\nu=x,y,z} \frac{\partial M_\nu}{\partial x_\mu}\frac{\partial M_\nu}{\partial x_\mu}. \tag{47}$$

This section not complete.

7.3 Quantum antiferromagnet

Antiferromagnetic systems are generally approached by analogy with ferromagnetic systems, assuming that the system can be divided up into two or more *sublattices*, i.e. infinite interpenetrating subsets of the lattice whose union is the entire lattice. Classically, it is frequently clear that if we choose all spins on a given judiciously chosen sublattice to be aligned with one another, we must achieve a minimum in the energy. For example, for the classical AF Heisenberg model $H = J\sum_{i\delta}\mathbf{S}_i \cdot \mathbf{S}_{i+\delta}$ with $J > 0$ on a square lattice, choosing the A-B sublattices in the figure and making all spins up on one and down on another allows each bond to achieve its lowest energy of $-JS^2$. This state, with alternating up and down spins, is referred to as the classical Neél state. Similarly, it may be clear to you that on the triangular lattice the classical lowest energy configuration is achieved when spins are placed at 120° with respect to one another on the sublattices A, B, C. However, quantum magnetic systems are not quite

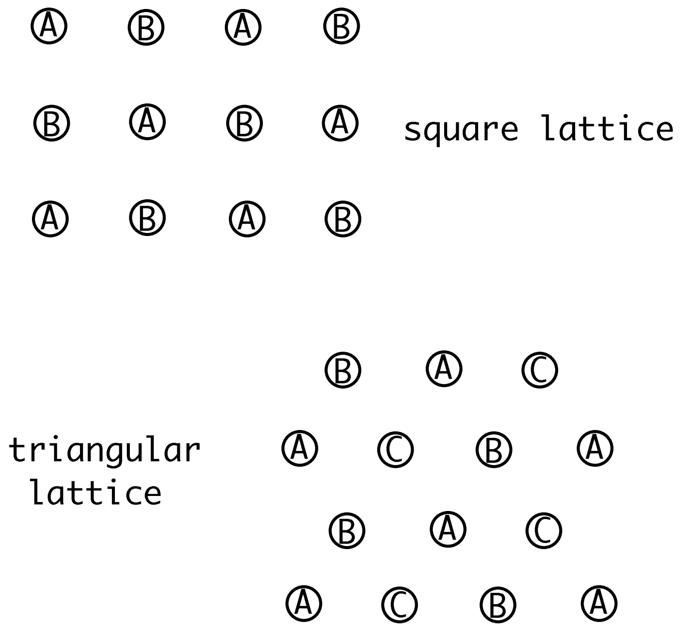


Figure 5: Possible choice of sublattices for antiferromagnet

so simple. Consider the magnetization M_A on a given sublattice (say the A sites in the figure) of the square lattice; alternatively one can define the *staggered magnetization* as $M_s = \Sigma_i (-1)^i \langle \hat{\mathbf{S}}_i \rangle$ (Note $(-1)^i$ means $+1$ on the A sites and -1 on the B sites.) Either construct can be used as the order parameter for an antiferromagnet on a bipartite lattice. In the classical Neél state, these is simply $M_A = NS/2$ and $M_s = NS$, respectively, i.e. the sublattice or staggered magnetization are saturated. In the wave function for the ground state of a *quantum* Heisenberg antiferromagnet, however, there is some amplitude for spins to be flipped on a a given sublattice, due to the fact that for a given bond the system can lower its energy by taking advantage of the $\hat{S}_x \hat{S}'_x + \hat{S}_y \hat{S}'_y$ terms. This effect can be seen already by examining the two-spin 1/2 case for the ferromagnet and antiferromagnet. For the ferromagnet, the classical energy is $-|J|S^2 = -|J|/4$, but the quantum energy in the total spin

1 state is also $-|J|/4$. For the antiferromagnet, the classical energy is $-JS^2 = -J/4$, but the energy in the total spin 0 quantum mechanical state is $-3J/4$. So quantum fluctuations–which inevitably depress the magnetization on a given sublattice–lower the energy in the antiferromagnetic case. This can be illustrated in a very simple calculation of magnons in the antiferromagnet following our previous discussion in section 7.2.

7.3.1 Antiferromagnetic magnons

We will follow the same procedure for the ferromagnet on each sublattice A and B, defining

$$\begin{aligned}
\hat{S}_i^{A+} &= \hat{S}_{ix}^A + i\hat{S}_{iy}^A = (2S)^{1/2}\left(1 - \frac{A_i^\dagger A_i}{2S}\right)^{1/2} A_i && (48)\\
\hat{S}_i^{A-} &= \hat{S}_{ix}^A - i\hat{S}_{iy}^A = (2S)^{1/2} A_i^\dagger \left(1 - \frac{A_i^\dagger A_i}{2S}\right)^{1/2} && (49)\\
\hat{S}_i^{B+} &= \hat{S}_{ix}^B + i\hat{S}_{iy}^B = (2S)^{1/2}\left(1 - \frac{B_i^\dagger B_i}{2S}\right)^{1/2} B_i && (50)\\
\hat{S}_i^{B-} &= \hat{S}_{ix}^B - i\hat{S}_{iy}^B = (2S)^{1/2} B_i^\dagger \left(1 - \frac{B_i^\dagger B_i}{2S}\right)^{1/2} && (51)\\
S_{iz}^A &= S - A_i^\dagger A_i && (52)\\
-S_{iz}^B &= S - B_i^\dagger B_i, && (53)
\end{aligned}$$

i.e. we assume that in the absence of any quantum fluctuations spins on sublattice A are up and those on B are down. Otherwise the formalism on each sublattice is identical to what we did for the ferromagnet. We introduce on each sublattice creation & annihilation operators for spin waves with momentum $\mathbf{k}$:

$$a_{\mathbf{k}} = \frac{1}{N^{1/2}} \sum_{i \in A} A_i e^{i\mathbf{k}\cdot\mathbf{R}_i}; \qquad a_{\mathbf{k}}^\dagger = \frac{1}{N^{1/2}} \sum_{i \in A} A_i^\dagger e^{-i\mathbf{k}\cdot\mathbf{R}_i} \qquad (54)$$

$$b_{\mathbf{k}} = \frac{1}{N^{1/2}} \sum_{i \in B} B_i e^{i\mathbf{k}\cdot\mathbf{R}_i}; \qquad b_{\mathbf{k}}^\dagger = \frac{1}{N^{1/2}} \sum_{i \in B} B_i^\dagger e^{-i\mathbf{k}\cdot\mathbf{R}_i}. \tag{55}$$

In principle $\mathbf{k}$ takes values only in the 1st *magnetic Brillouin zone*, or *half-zone*, since the periodicity of the sublattices is twice that of the underlying lattice. The spin operators on a given site are then expanded as

$$\hat{S}_i^{A+} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}} + \ldots\right], \tag{56}$$

$$\hat{S}_i^{B+} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_i} b_{\mathbf{k}} + \ldots\right], \tag{57}$$

$$\hat{S}_i^{A-} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} a_{\mathbf{k}}^\dagger + \ldots\right], \tag{58}$$

$$\hat{S}_i^{B-} \simeq \left(\frac{2S}{N}\right)^{1/2} \left[\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} b_{\mathbf{k}}^\dagger + \ldots\right], \tag{59}$$

$$\hat{S}_{iz}^{A} = S - \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'} \tag{60}$$

$$\hat{S}_{iz}^{B} = -S + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} a_{\mathbf{k}}^\dagger a_{\mathbf{k}'}. \tag{61}$$

The expansion of the Heisenberg Hamiltonian in terms of these variables is now (compare (36))

$$H = -NzJS^2 + H_0^{magnon} + \mathcal{O}(1), \tag{62}$$

$$H_0^{magnon} = JzS \sum_{\mathbf{k}} \left[\gamma_{\mathbf{k}}(A_{\mathbf{k}}^\dagger B_{\mathbf{k}}^\dagger + A_{\mathbf{k}} B_{\mathbf{k}}) + (A_{\mathbf{k}}^\dagger A_{\mathbf{k}} + B_{\mathbf{k}}^\dagger B_{\mathbf{k}})\right] \tag{63}$$

Unlike the ferromagnetic case, merely expressing the Hamiltonian to bilinear order in the magnon variables does not diagonalize it immediately. We can however perform a canonical transformation[20] to bring the Hamiltonian into diagonal form (check!):

$$\alpha_{\mathbf{k}} = u_{\mathbf{k}} A_{\mathbf{k}} - v_{\mathbf{k}} B_{\mathbf{k}}^\dagger \; ; \quad \alpha_{\mathbf{k}}^\dagger = u_{\mathbf{k}} A_{\mathbf{k}}^\dagger - v_{\mathbf{k}} B_{\mathbf{k}} \tag{64}$$

[20] The definition of a canonical transformation, I remind you, is one which will give canonical commutation relations for the transformed fields. This is important because it ensures that we can interpret the Hamiltonian represented in terms of the new fields as a (now diagonal) fermion Hamiltonian, read off the energies, etc.

$$\beta_{\mathbf{k}} = u_{\mathbf{k}} B_{\mathbf{k}} - v_{\mathbf{k}} A^{\dagger}_{\mathbf{k}} \; ; \quad \beta^{\dagger}_{\mathbf{k}} = u_{\mathbf{k}} B^{\dagger}_{\mathbf{k}} - v_{\mathbf{k}} A_{\mathbf{k}}, \tag{65}$$

where the coefficients $u_{\mathbf{k}}, v_{\mathbf{k}}$ must be chosen such that $u^2_{\mathbf{k}} - v^2_{\mathbf{k}} = 1$. One such choice is $u_{\mathbf{k}} = \cosh\theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh\theta_{\mathbf{k}}$. For each $\mathbf{k}$, choose the angle $\theta_{\mathbf{k}}$ such that the anomalous terms like $A^{\dagger}_{\mathbf{k}} B^{\dagger}_{\mathbf{k}}$ vanish. One then finds the solution

$$\tanh 2\theta_{\mathbf{k}} = -\gamma_{\mathbf{k}}, \tag{66}$$

and

$$H_0^{magnon} = -NE_J + \sum_{\mathbf{k}} \omega_{\mathbf{k}} (\alpha^{\dagger}_{\mathbf{k}} \alpha_{\mathbf{k}} + \beta^{\dagger}_{\mathbf{k}} \beta_{\mathbf{k}} + 1), \tag{67}$$

where

$$\omega^2_{\mathbf{k}} = E^2_J (1 - \gamma^2_{\mathbf{k}}), \tag{68}$$

and $E_J = JzS$. Whereas in the ferromagnetic case we had $\omega_{\mathbf{k}} \sim (1 - \gamma_{\mathbf{k}}) \sim k^2$, it is noteworthy that in the antiferromagnetic case the result $\omega_{\mathbf{k}} \sim (1-\gamma_{\mathbf{k}})^{1/2} \sim k$ gives a linear magnon dispersion at long wavelengths (a center of symmetry of the crystal must be assumed to draw this conclusion). Note further that for each $\mathbf{k}$ there are two degenerate modes in H_0^{magnon}.

7.3.2 Quantum fluctuations in the ground state

check factors of 2 from def. of N, J

At $T = 0$, there are no thermally excited spin wave excitations. Nevertheless the spin wave theory yields an decrease of the ground state energy relative to the classical value $-NJzS^2$, but an *increase* over the quantum ferromagnet result of $-N|J|S(S+1)$ due to the zero-point (constant)

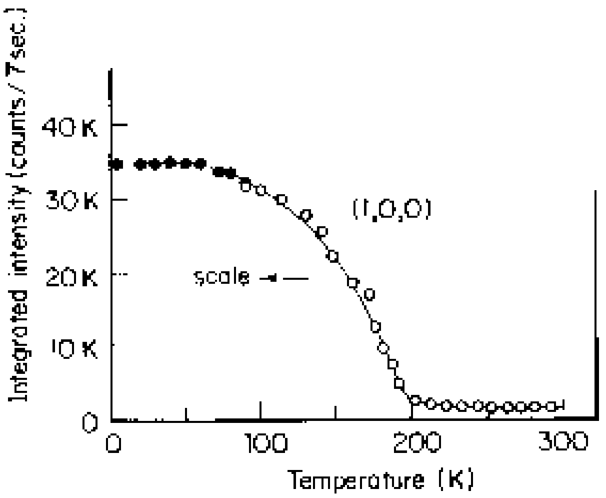


Figure 6: Integrated intensity of (100) Bragg peak vs. temperature for $LaCuO_4$, with $T_N = 195K$. (After Shirane et al. 1987)

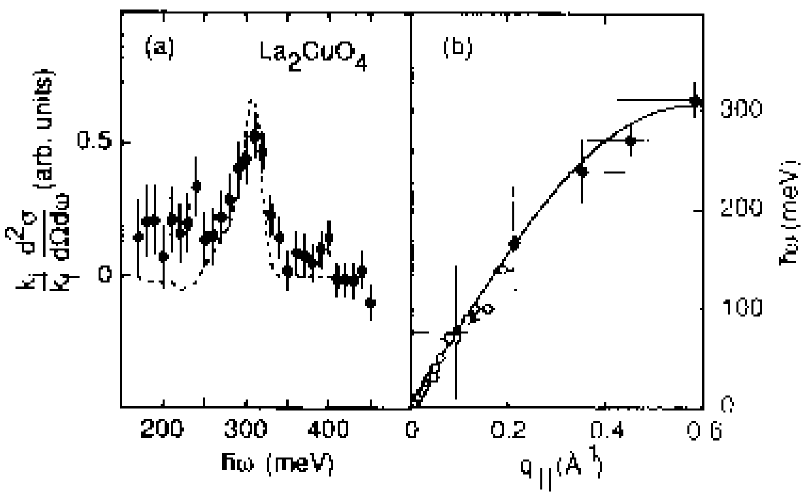


Figure 7: a) Inelastic neutron scattering intensity vs. energy transfer at 296K near zone boundary $Q = (1, k, 0.5)$ for oriented $LaCuO_4$ crystals with Neél temperature 260K; b) spin-wave dispersion $\omega_{\mathbf{q}}$ vs. $q_{\|}$, where $q_{\|}$ is in-plane wavevector. (after Hayden et al. 1991)

term in (67).[21] The ground-state energy is

$$E_0 \simeq -NE_J + \sum_{\mathbf{k}} \omega_{\mathbf{k}}. \tag{69}$$

The result is usually expressed in terms of a constant β defined by

$$E_0 \equiv -NJzS\left(S + \frac{\beta}{z}\right), \tag{70}$$

and $\beta = 0.58$ for 3D and xxx for 2D.

Quantum fluctuations have the further effect of preventing the staggered magnetization from achieving its full saturated value of S, as in the classical Neél state, as shown first by Anderson.[22] Let us consider the average z-component of spin in equilibrium at temperature T, averaging only over spins on sublattice A of a D-dimensional hypercubic lattice. From (60), we have $\langle \hat{S}_z^A \rangle = S - N^{-1}\sum_{\mathbf{k}}\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle$ within linear spin wave theory. Inverting the transformation (65), we can express the A's in terms of the α's and β's, whose averages we can easily calculate. Note the 0th order in $1/S$ gives the classical result, $\langle \hat{\mathbf{S}}_z^A \rangle$, and the deviation is the spin wave reduction of the sublattice moment

$$\begin{aligned}
\frac{\delta M_A}{N} &= \langle \hat{S}_z^A \rangle - S = -\frac{1}{N}\sum_k \langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle \\
&= -\frac{1}{N}\sum_{\mathbf{k}} \langle (u_{\mathbf{k}}\alpha_{\mathbf{k}}^\dagger + v_{\mathbf{k}}\beta_{\mathbf{k}})(u_{\mathbf{k}}\alpha_{\mathbf{k}} + v_{\mathbf{k}}\beta_{\mathbf{k}}^\dagger)\rangle \\
&= -\frac{1}{N}\sum_{\mathbf{k}} u_{\mathbf{k}}^2\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}\rangle + v_{\mathbf{k}}^2\langle \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}\rangle,
\end{aligned} \tag{71}$$

where N is the number of spins on sublattice B. We have neglected cross terms like $\langle \alpha_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}^\dagger \rangle$ because the α and β are independent quanta by construction. However the diagonal averages $\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}\rangle$ and $\langle \beta_{\mathbf{k}}^\dagger \beta_{\mathbf{k}}\rangle$ are the expectation values for the number operators of independent bosons with dispersion $\omega_{\mathbf{k}}$ in equiblibrium, and so can be replaced (within linear spin

[21] Recall the classical Neél state, which does not contain such fluctuations, is *not* an eigenstate of the quantum Heisenberg Hamiltonian.

[22] P.W. Anderson, Phys. Rev. 86, 694 (1952).

wave theory) by

$$n_{\mathbf{k}} \equiv \langle \beta^{\dagger}_{\mathbf{k}} \beta_{\mathbf{k}} \rangle = \langle \alpha^{\dagger}_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle = b(\omega_{\mathbf{k}}), \tag{72}$$

where b is the Bose distribution function. The tranformation coefficients $u_{\mathbf{k}} = \cosh \theta_{\mathbf{k}}$ and $v_{\mathbf{k}} = \sinh \theta_{\mathbf{k}}$ are determined by the condition (66) such that

$$u^2_{\mathbf{k}} + v^2_{\mathbf{k}} = \cosh 2\theta_{\mathbf{k}} = \frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}} \tag{73}$$

$$v^2_{\mathbf{k}} = \frac{1}{2}\left(\frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}} - 1 \right), \tag{74}$$

such that the sulattice magnetization (71) becomes

$$\boxed{\frac{\delta M_A}{N} = \frac{1}{2} - \frac{1}{N}\sum_{\mathbf{k}} \left(n_{\mathbf{k}} + \frac{1}{2} \right) \frac{1}{\sqrt{1-\gamma^2_{\mathbf{k}}}}} \tag{75}$$

<u>Remarks:</u>

1. The correction δM_A is independent of S, and negative as it must be (see next point). However relative to the leading classical term S it becomes smaller and smaller as S increases, as expected.

2. The integral in (75) depends on the dimensionality of the system. It has a T-dependent part coming from $n_{\mathbf{k}}$ and a T-independent part coming from the $1/2$. At $T = 0$, where there are no spin waves excited thermally, $n_{\mathbf{k}} = 0$, and we find

$$\frac{\delta M_A}{N} \simeq \begin{cases} -0.078 & D = 3 \\ -0.196 & D = 2 \\ \infty & D = 1 \end{cases} \tag{76}$$

   The divergence in $D = 1$ indicates the failure of spin-wave theory in one dimension, as discussed further in section xxx.

3. The low temperature behavior of $\delta M(T)$ must be calculated carefully due to the singularities of the bose distribution function when $\omega_k \to 0$. If this divergence is cut off by introducing a scale k_0 near $\mathbf{k} = 0$ and $\mathbf{k} = (\Pi/a, \Pi/a)$, one finds that δM_A diverges as $1/k_0$ in 1D, and as $\log k_0$ in 2D, whereas it is finite as $\mathbf{k}_0 \to 0$ in 3D. Thus on this basis one does not expect long range spin order at any nonzero temperature in two dimensions (see discussion of Mermin-Wagner theorem below), nor even at $T = 0$ in one dimension.

7.3.3 Nonlinear spin wave theory

7.3.4 Frustrated models

7.4 1D & 2D Heisenberg magnets

7.4.1 Mermin-Wagner theorem

7.4.2 1D: Bethe solution

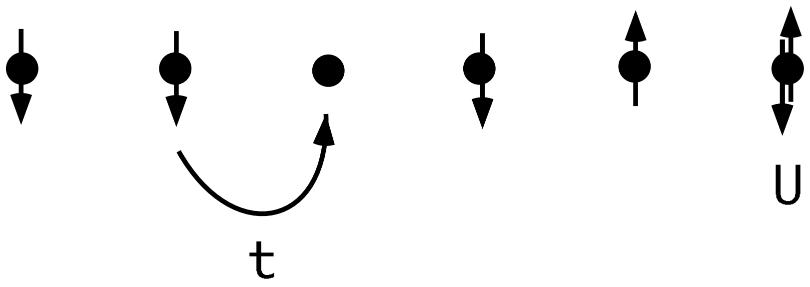
7.4.3 2D: Brief summary

7.5 Hubbard model and itinerant magnetism

I want to show you one more example of the use of the RPA, to describe the approach to a phase transition. A great deal of attention has been focussed on the Hubbard model and its variants, particularly because it is the simplest model known to display a metal-insulator (Mott-Hubbard) transition qualitatively similar to what is observed in the high temperature superconductors. The Hubbard model consists of a lattice of sites labelled by i, on which electrons of spin $\uparrow$ or $\downarrow$ may sit. The kinetic energy term in the Hamiltonian allows for electrons to hop between sites with matrix element t, and the potential energy simply requires an energy cost U every time two opposing spins occupy the same site.[23] Longer range interactions are neglected:

$$H = -t \sum_{\substack{\sigma \\ <i,j>}} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} U \sum_{\sigma} n_{i\sigma} n_{i-\sigma}, \qquad (77)$$

where $< ij >$ means nearest neighbors only.



In its current form the kinetic energy, when Fourier transformed, corresponds, to a tight binding band in d dimensions of width 4dt,

$$\epsilon_k = -2t \sum_{\alpha=1}^{d} \cos k_\alpha a, \qquad (78)$$

where a is the lattice constant. The physics of the model is as follows. Imagine first that there is one electron per site, i.e. the band is half-filled. If $U = 0$ the system is clearly metallic, but if $U \to \infty$, double occupation of sites will be "frozen out". Since there are no holes, electrons cannot move, so the model must correspond to an insulating state; at some critical U a metal-insulator transition must take place. We are more interested in the case away from half-filling, where the Hubbard model is thought for large U and small doping (deviation of density from 1 particle/site) to have a ferromagnetic ground state.[24] In particular, we would like to

[23]What happened to the long-range part of the Coulomb interaction? Now that we know it is screened, we can hope to describe its effects by including only its matrix elements between electrons in wave functions localized on site i and site j, with $|i-j|$ smaller than a screening length. The largest element is normally the $i=j$ one, so it is frequently retained by itself. Note the Hamiltonian (77) includes only an on-site interaction for opposite spins. Of course like spins are forbidden to occupy the same site anyway by the Pauli principle.

[24]At 1/2-filling, one electron per site, a great deal is known about the Hubbard model, in particular that the system is metallic for small U (at least for non-nested lattices, otherwise a narrow-gap spin density wave instability is present), but that as we increase U past a critical value $U_c \sim D$ a transition to an antiferromagnetic insulating state occurs (Brinkman-Rice transition). With one single hole present, as $U \to \infty$, the system is however ferromagnetic (Nagaoka state).

investigate the transition from a *paragmagnetic* to a *ferromagnetic* state as T is lowered.

This instability must show up in some quantity we can calculate. In a ferromagnet the susceptibility χ diverges at the transition, i.e. the magnetization produced by the application of an infinitesimal external field is suddenly finite. In many-body language, the static, uniform spin susceptibility is the retarded spin density – spin density correlation function,

$$\chi = \chi(q=0,\omega=0) = \lim_{h_z\to 0}\frac{\langle S_z\rangle}{h_z} = \int d^3r \int_0^\infty dt \langle [S_z(r,t), S_z(0,0)]\rangle, \tag{79}$$

where in terms of electron number operators $n_\sigma = \psi_\sigma^\dagger \psi_\sigma$, the magnetization operators are $S_z = (1/2)[n_\uparrow - n_\downarrow]$, i.e. they just measure the surplus of up over down spins at some point in space.

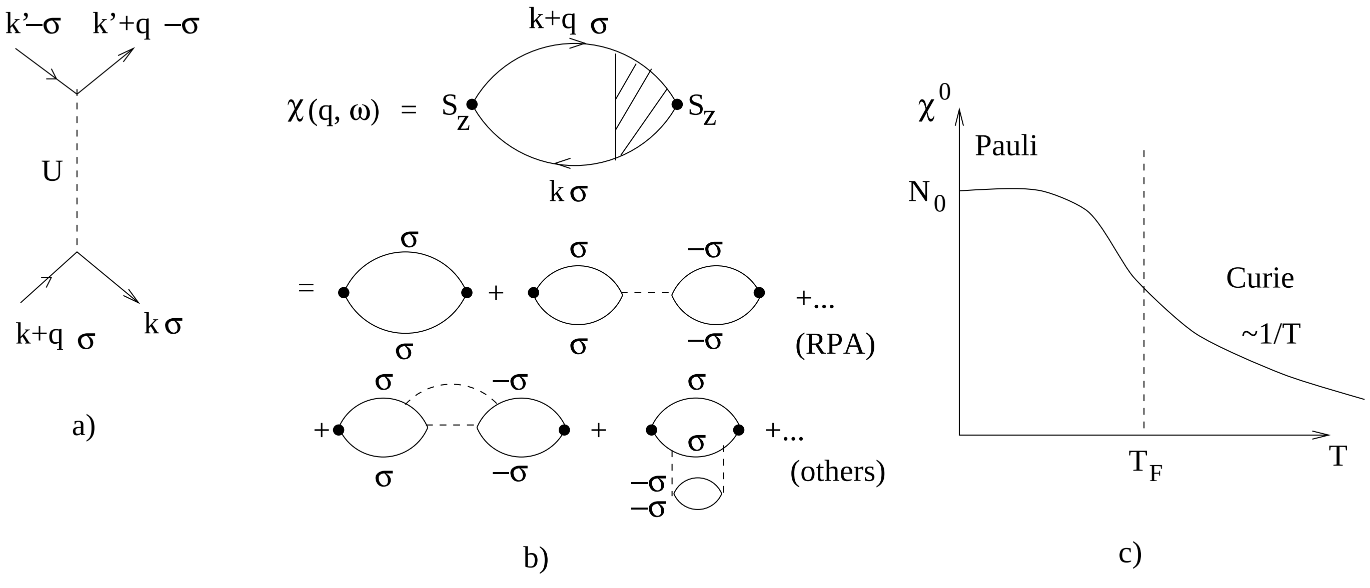


Figure 8: 1a) Hubbard interaction; 1b) Spin suceptibility perturbation series; 1c) Spin susceptibility vs. T for free fermions.

Diagramatically, the Hubbard interaction $H_{int} = U\,\Sigma_i\, n_{i\uparrow} n_{i\downarrow}$ looks like figure 8a); note only Green's function lines of opposite spins interact. The magnetic susceptibility is a correlation function similar to the charge susceptibility we have already calculated, and is therefore represented by Fig. 8b). At time t=0, we measure the magnetization S_z of the system, allow the particle and hole thus created to propagate to a later time, scatter in all possible ways, and remeasure S_z. The so-called "Stoner model" of ferromagnetism approximates the perturbation series by the RPA sum[25] we have already encountered,[26] which gives $\chi = \chi_0/(1-U\chi_0)$. At sufficiently high T (χ_0 varies as $1/T$ in the nondegenerate regime, Fig. 8c)) we will have $U\chi_0(T) < 1$, but as T is lowered, $U\chi_0(T)$ increases. If U is large enough, such that $UN_0 > 1$, there will be a transition at $U\chi_0(T_c) = 1$, where χ diverges. Note for $U\chi_0(T) > 1$ ($T < T_c$), the susceptibility is negative, so the model is unphysical in this region. This problem arises in part because the ferromagnetic state has a spontaneously broken symmetry, $\langle S_z \rangle \neq 0$ even for $h_z \to 0$, and the calculation we did implicitly assumed a paramagnetic state, e.g. $G^0_\sigma = G^0_{-\sigma}$. Nevertheless the approach to the transition from above and the location of the transition appear qualitatively reasonable.

7.5.1 Moment formation in itinerant systems

7.5.2 Kondo model

[25]What justifies throwing away other diagrams in this case?
[26]In the static, homogeneous case it is equivalent to the self-consistent field method of Weiss.