TA1 THEORETICAL SOLID STATE PHYSICS WS2016-17

1. Second quantization giamarchi [2]

1.1. Bosons.

$$a_i^\dagger |n_1, \dots, n_i, \dots, n_\Omega\rangle = \sqrt{n_i + 1}|n_1, \dots, n_i + 1, \dots, n_\Omega\rangle$$
$$a_i |n_1, \dots, n_i, \dots, n_\Omega\rangle = \sqrt{n_i}|n_1, \dots, n_i - 1, \dots, n_\Omega\rangle$$

Vacuum

$$|\emptyset\rangle = |n_1 = 0, n_2 = 0, \dots, n_\Omega = 0\rangle.$$

Then

$$|n_1, \dots, n_\Omega\rangle = \frac{1}{\sqrt{n_1!} \cdots \sqrt{n_\Omega!}} (a_1^\dagger)^{n_1} \cdots (a_\Omega^\dagger)^{n_\Omega} |\emptyset\rangle.$$

$$a_i^\dagger a_i |n_1, \dots, n_i, \dots, n_\Omega\rangle = n_i |n_1, \dots, n_i, \dots, n_\Omega\rangle$$

$$[a_i^\dagger, a_j^\dagger] = 0$$
$$[a_i, a_j] = 0$$
$$[a_i, a_j^\dagger] = \delta_{ij}$$

1.2. Fermions.

$$c_i^\dagger |n_1, \dots, n_i, \dots, n_\Omega\rangle = (1 - n_i)(-1)^{\varepsilon_i} |n_1, \dots, n_i + 1, \dots, n_\Omega\rangle$$
$$c_i |n_1, \dots, n_i, \dots, n_\Omega\rangle = n_i (-1)^{\varepsilon_i} |n_1, \dots, n_i - 1, \dots, n_\Omega\rangle,$$

where $\varepsilon_i := \sum_{j=1}^{i-1} n_j$, $\varepsilon_1 = 0$.

Then for $n_i \in \{0, 1\}$,

$$|n_1, \dots, n_\Omega\rangle = (c_1^\dagger)^{n_1} \cdots (c_\Omega^\dagger)^{n_\Omega} |\emptyset\rangle.$$

$$c_i^\dagger c_i |n_1, \dots, n_i = 0, \dots, n_\Omega\rangle = 0$$
$$c_i c_i^\dagger |n_1, \dots, n_i = 0, \dots, n_\Omega\rangle = |n_1, \dots, n_i = 0, \dots, n_\Omega\rangle$$

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

Short note: Use tensor product to determine if things are orthogonal.

2. Hartree-Fock

TODO Hartree-Fock; see also MQM notes

Date: March 5, 2017.

3. Dielectric response and the Lindhard function [after [4, Ch.3]]

We switch on a potential adiabatically ($\eta \searrow 0$). For simplicity, we only switch on a single Fourier component,

$$V_a(r,t) = V_a(q,\omega)e^{iq\cdot r - i\omega t}e^{\eta t}.$$

From linear response theory, we obtain the change in electron density,

$$\delta n_{\text{ind}}(q,\omega) = \chi_0(q,\omega)V_a(q,\omega),$$

where $\chi_0(q,\omega)$ is the *Lindhard function*

$$\chi_0(q,\omega) = \frac{1}{V}\sum_{k,s}\frac{n_{k+q,s} - n_{k,s}}{\mathcal{E}_{k+q} - \mathcal{E}_k - \hbar(\omega + i\eta)}. \tag{3.1}$$

The function $n_{k,s}$ is the electron density, for us usually we ignore s, and then use the Fermi function

$$n_k = \frac{1}{\exp[(\mathcal{E}_k - \mathcal{E}_F)/(k_B T)] + 1}.$$

The *dielectric function* ε is

$$\varepsilon(q,\omega) := 1 - \frac{4\pi e^2}{q^2}\chi_0(q,\omega). \tag{3.2}$$

It has something to do with renormalizing the external potential.

In the Thomas-Fermi limit, we take $\omega \to 0$ (static field) and a continuum limit. Taylor expanding $\mathcal{E}_k$ and n_k for $|q| \ll k_F$, we can obtain

$$\chi_0(q,0) \approx \int_{1BZ}\frac{dk}{4\pi^2}\frac{\partial n_k}{\partial \mathcal{E}_k} = \frac{\partial n}{\partial \mathcal{E}_k},$$

where $n = N/V$ is the particle density. Thus for the dielectric function, we have

$$\varepsilon(q) \approx 1 + \frac{4\pi e^2}{q^2}\frac{\partial n}{\partial \mathcal{E}_k}.$$

4. Magnetism [am [1, Ch.33]]

Consider two adjacent spin-S spins, and let $S_1 \equiv S_1 \otimes I$ and $S_2 \equiv I \otimes S_2$ be their spin operators (which measure spin). Recall the S_i are ("vector-valued") of the form $S = (S_x, S_y, S_z) = \frac{1}{2}\sigma$. A basis for the Hilbert space of these two spin particles is given by the $(2S+1)^2$ vectors $|s_1 s_1^z, s_2 s_2^z\rangle$, which are eigenfunctions of S^2 and S^z (recall $[S^2, S^z] = 0$):

$$\begin{aligned} S_i^2|s_1 s_1^z, s_2 s_2^z\rangle &= s_i(s_i+1)|s_1 s_1^z, s_2 s_2^z\rangle \\ S_i^z|s_1 s_1^z, s_2 s_2^z\rangle &= s_i^z|s_1 s_1^z, s_2 s_2^z\rangle. \end{aligned}$$

This is called the *product* basis; they have well-defined S^2 and S^z for *individual* spins. For some reason we leave s_i in there even though $s_1 = s_2 = S$. On the other hand, s_i^z ranges through the $2S+1$ values $\{-s_i, -s_i+1, \ldots, s_i - 1, s_i\}$.

Define the *total spin operator* $S := S_1 + S_2$, so e.g. $S^z = S_1^z + S_2^z$ and $S^2 = (S_1+S_2)^2 = S_1^2 + S_2^2 + 2S_1\cdot S_2$. The new S^z still has the product basis as eigenvectors. However, S^2 does not, because of the $S_1 \cdot S_2$ term. (It does not commute with S_i^z.) The matrix elements of S^2 on the product basis can be computed using e.g.

$$S_1 \cdot S_2 = S_1^z S_2^z + \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+),$$

where $S_{i\pm} = S_i^x \pm S_i^y$. A basis for S^2 and S^z is called the *total-s* basis.

4.1. Spin-1/2 particles.

In this case there are four product basis vectors $|1/2\ \pm 1/2, 1/2\ \pm 1/2\rangle$. The total-$s$ basis is

$$\begin{aligned} |s=1\ s^z=1\rangle &= |++\rangle \\ |s=1\ s^z=0\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \\ |s=1\ s^z=-1\rangle &= |--\rangle \\ |s=0\ s^z=0\rangle &= \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle). \end{aligned}$$

They split into a *spin singlet* with $S = S^z = 0$,

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle),$$

and *spin triplets*

$$\begin{array}{ll} |\uparrow\uparrow\rangle & S=1,\ S^z=1 \\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) & S=1,\ S^z=0 \\ |\downarrow\downarrow\rangle & S=1,\ S^z=1 \end{array}$$

4.2. **Heisenberg model.** Now we go to more than 2 particles, but still only two-particle interactions. The *Heisenberg model* consists of a large lattice of magnetic ions with nearest neighbor interactions and a constant magnetic field $H = H\widehat{z}$, with spin Hamiltonian

$$H = -\sum_{\langle ll'\rangle} J_{ll'} S_l \cdot S_{l'} - h\sum_l S_l^z \tag{4.1}$$

eqn:pm

$$= -\sum_{\langle ll'\rangle} J_{ll'}(S_l^z S_{l'}^z + \frac{1}{2}(S_l^+ S_{l'}^- + S_{l'}^+ S_l^-)) - h\sum_l S_l^z, \tag{4.2}$$

where

$$S^{\pm} := S^x \pm iS^y,$$

called raising and lowering operators. The raising and lowering operators satisfy

$$S^{\pm}|S, S^z\rangle = \sqrt{(S \mp S^z)(S + 1 \pm S^z)}|S, S^z \pm 1\rangle.$$

In particular, $S^+|S, S\rangle = 0$, and $S^-|S, -S\rangle = 0$.

Note the interaction $J_{ll'}$ may depend on the spin pair that is interacting. This is called the *isotropic* case since the $J_{ll'}$ is the same on the z-part, $S_1^z S_2^z$, as on the x and y parts, $\frac{1}{2}(S_1^+ S_2^- + S_2^+ S_1^-)$. The *anisotropic* ferromagnetic case, where we have a $J_{ll'}^z > J_{ll'} > 0$ will be analyzed in a homework exercise.

4.2.1. *Ground state.* The ground state of the Heisenberg *ferromagnet* (all $J_{ll'} \geq 0$) is easy to find. In the classical case it is simply the state with all spins pointing in the z direction (for $h > 0$), i.e. $|\uparrow\uparrow\uparrow\cdots\uparrow\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes \cdots \otimes |\uparrow\rangle$. This suggests for the quantum case, that we also choose all the spins to be aligned in the z-axis (with the magnetic field h). We guess it is

$$|0\rangle := |S\rangle \otimes \cdots \otimes |S\rangle = \prod_l |S\rangle,$$

where in product basis $|S\rangle = |S, S\rangle$, i.e. an eigenstate of S^z with maximum eigenvalue S. This is an eigenvector, as in (4.2), the term $S_l^+|S\rangle = 0$. It has energy

$$E_0 = -S^2 \sum_{\langle ll'\rangle} J_{ll'} - NhS.$$

We show this is the minimum energy. Since all $J_{ll'} \geq 0$, then for $\|\psi\| = 1$,

$$\begin{aligned} \langle\psi|H|\psi\rangle &\geq -\sum_{\langle ll'\rangle} J_{ll'} \max_{\|\psi\|=1} \langle S_l \cdot S_{l'}\rangle - h\sum_l \max_{\|\psi\|=1} \langle S_l^z\rangle \\ &\geq -S^2 \sum_{\langle ll'\rangle} J_{ll'} - NhS, \end{aligned}$$

using

$$\begin{aligned} \max\langle S_l \cdot S_{l'}\rangle &\leq S^2 \\ \max\langle S_l^z\rangle &\leq S. \end{aligned}$$

These inequalities follow, from the fact that the maximum $\langle\psi|A|\psi\rangle$ with $\|\psi\| = 1$ is equal to the largest eigenvalue of A, and that $-2S_l \cdot S_{l'} = (S_l + S_{l'})^2 - S_l^2 - S_{l'}^2$. In fact, we even know the maximum here is attained for $\prod_l |S\rangle$.

The ground state of the Heisenberg *antiferromagnet* (some $J < 0$) is much harder to determine, as states like $|\uparrow\downarrow\uparrow\cdots\rangle$, which would work in the classical case, are not eigenstates of the Hamiltonian. In the ferromagnet, $S_-(R)S_+(R')|0\rangle = 0$, which is not the case for the ferromagnet. In 1D or when J is a constant, the ground state was determined by Bethe (1931).

4.3. **Spin waves and low T in the Heisenberg model.** Many low-energy excitation of the Heisenberg ferromagnet are *spin waves*, where the spin orientation slowly rotates as one moves through the lattice. These are also called *magnons*.

In the *Schwinger representation*, the Heisenberg Hamiltonian (for both ferromagnet and antiferromagnet) is written in terms of Bose operators.

TODO schwinger

Let $\mathcal{E}(k) := E_k - E_0$. The excitation energy of an excited state constructed by superposition of spin waves is

$$\sum \mathcal{E}(k) n_k, \qquad n_k = 0, 1, 2, \dots,$$

where n_k is the number of spin waves with wave vector k. The expected value, just as for phonons, is given by the Bose distribution,

$$\langle n_k \rangle = \frac{1}{e^{\mathcal{E}(k)/(k_B T)} - 1}.$$

As each spin wave decreases the total spin by one unit, the magnetization at temperature T is

$$M(T) = M(0) - \sum_k \langle n_k \rangle \tag{4.3}$$

eqn:M

$$\approx M(0) \left[1 - \frac{V}{NS} \int_{1BZ} \frac{d^3k}{(2\pi)^3} \frac{1}{(e^{\mathcal{E}(k)/(k_B T)} - 1)} \right]. \tag{4.4}$$

Note $M(0) = NS$ since there are N spins, and in the ground state they all have mean spin S.

The *spontaneous* magnetization is described by $M(T)$ in the limit as external magnetic field $h \to 0$. TODO explain (AM):

$$\mathcal{E}(k) = E_k - E_0 = 2S \sum_R J(R) \sin^2(\frac{1}{2} k \cdot R) + h. \tag{4.5}$$

As $T \to 0$, only spin waves with small k with contribute to the integral in M, so

$$\mathcal{E}(k) \approx \frac{S}{2} \sum_R J(R) (k \cdot R)^2.$$

We plug this into (4.4) and make the substitution $q := (k_B T)^{-1/2} k$ to cancel the $k_B T$ in the Bose factor; then we obtain

eqn:M2

$$M(T) = M(0) \left[1 - \frac{V}{NS} (k_B T)^{3/2} \int \frac{dq}{(2\pi)^3} \frac{1}{\exp(\frac{S}{2} \sum_R J(R)(q \cdot R)^2) - 1} \right]. \tag{4.6}$$

The behavior $M(T) \sim T^{3/2}$ for low T is called the *Bloch $T^{3/2}$ law*, and agrees with experiment.

Remark. In dimensions 1 and 2, the integral in (4.6) diverges like $\int \frac{1}{q^2}$ as $q \to 0$. The interpretation is that for $T \neq 0$, there are so many spin waves excited that there is no magnetization. Thus there is *no spontaneous magnetization* in isotropic Heisenberg model in 1 or 2 dimensions.

4.3.1. *Spin waves in antiferromagnets.* The Néel state is the state where neighboring spins are oppositely oriented. This is not the ground state, but at least is an approximate solution. We can transform the Hamiltonian to make computations involving the Néel state easier. By rotating all the spin operators on one sublattice around the x-axis, we send

$$S^{\pm}_{l'} \mapsto S^{\mp}_{l'}, \qquad S^z_{l'} \mapsto -S^z_{l'}.$$

The resulting Hamiltonian on the ferromagnetic ground state (all spins in the same direction) then has the same energy as the Néel state with the original Hamiltonian.

4.4. **Hubbard model** marder [3]**.** This is an extension of the tight-binding model. There is energy penalty U for electrons on the same physical site. The Hubbard Hamiltonian in second quantized form is

$$H = -t \sum_{\langle ll' \rangle, \sigma} (c^\dagger_{l\sigma} c_{l'\sigma} + c^\dagger_{l'\sigma} c_{l\sigma}) + U \sum_l c^\dagger_{l\uparrow} c_{l\uparrow} c^\dagger_{l\downarrow} c_{l\downarrow}. \tag{4.7}$$

The exact solution is known in 1 dimension (Lieb and Wu 1968). For 3 dimensions, we resort to mean field theory. The difficulty is the last term $n_{l\uparrow} n_{l\downarrow}$, which is quartic. The mean field theory ansatz is to write

$$n_{\ell\sigma} = n_\sigma + (n_{l\sigma} - n_\sigma),$$

where n_σ is the average number of spins in state σ on the lattice. Then we expand the Hamiltonian to quadratic order to obtain

$$H \approx -t \sum_{\langle ll' \rangle, \sigma} (c^\dagger_{l\sigma} c_{l'\sigma} + c^\dagger_{l'\sigma} c_{l\sigma}) + U \sum_l n_{l\uparrow} n_\downarrow + n_{l\downarrow} n_\uparrow - n_\uparrow n_\downarrow. \tag{4.8}$$

The Hamiltonian becomes diagonal in Fourier space,

$$H = \sum_{k\delta\sigma} (-t \cos(\delta \cdot k) c^\dagger_{k\sigma} c_{k\sigma} + U \sum_k n_{k\uparrow} n_\downarrow + n_{k\downarrow} n_\uparrow - n_\uparrow n_\downarrow, \tag{4.9}$$

where δ are the nearest-neighbor vectors.

In 2 and 3 dimensions, we only really know what happens at half-filling, when the number of electrons N equals half the number of lattice sites. At half-filling and for sufficiently large U, the ground state is antiferromagnetic. This leads to antiferromagnetic insulators, called *Mott-Hubbard* (or *Mott*) insulators.

4.5. **Critical phenomena.**

$$C_V = \frac{\partial U}{\partial T}, \qquad U = -\frac{\partial}{\partial \beta} \log Z.$$

Magnetic susceptibility

$$\chi = \left. \frac{\partial M}{\partial h} \right|_{h=0}$$

$$M(T) \sim (T_c - T)^\beta$$
$$\chi(T) \sim (T - T_c)^{-\gamma}$$
$$C_V(T) \sim (T - T_C)^{-\alpha}$$

Experimentally: β usually between 0.33 and 0.37. γ usually between 1.3 and 1.4. α usually ≤ 0.1.

References

[1] N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, Harcourt College Publishers (1976).

[2] T. Giamarchi, A. Iucci, and C. Berthod, *Introduction to Many Body physics* lecture notes, University of Geneva (2008-2013). http://dqmp.unige.ch/giamarchi/local/people/thierry.giamarchi/pdf/many-body.pdf

[3] M. P. Marder, *Condensed Matter Physics*, Wiley (2010).

[4] M. Sigrist, *Solid State Theory* lecture notes, ETH Zurich (2014). http://edu.itp.phys.ethz.ch/fs14/sst/Lecture-Notes.pdf