Chapter 6: Hubbard Model

- → RPA susceptibility for spin & Charge
- → Stoner instability
- → spin wave (magnon).

- → Hartree Fock Mean Field Theory
- → Ferromagnetism
- → Spin Density wave (Antiferromagnetism).

- → Mott AFM insulator (real space mean field theory)
- → Effective / Renormalized Hamiltonian
- → t-J model.

Refs:
G. Mahan (Chapter 6).
P. Fazekas (Chapter 4)
Jeno Solyom (vol 3, chapter 33).
P. Phillips.

We have seen in the Linear Response Theory chapter that the Thomas Fermi screening length $q_{TF}^{-1} \sim 0.2\text{-}0.6\, r_s$. This is to say the Coulomb interaction indeed becomes very short in the scale of interatomic distance in a metal due to charge screening. With this observation J Hubbard proposed a low-energy effective model in which the Coulomb interaction is only onsite, often denoted by U, where

$$U = \int d^3r\, d^3r' \, |\phi(r)|^2 \frac{1}{|r-r'|} |\phi(r')|^2 \quad \cdots (1)$$

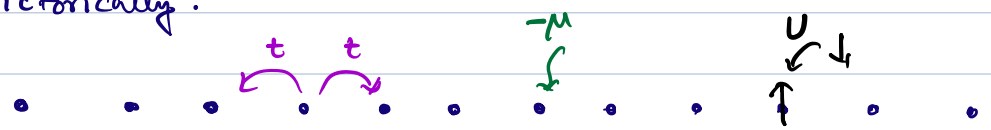
Since the interaction is strongest when two electrons are trying to be at the same site, and at the same site two electrons with opposite spins can only occupy due to the exclusion principle. Therefore, the lowest order effective model, as proposed by Hubbard, is

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} - \mu \sum_{i,\sigma} n_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \text{h.c.} \quad \cdots (2)$$

where $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$, and $\langle ij \rangle$ corresponds to nearest neighbor hopping.

- Clearly, the model can be easily generalized to next-nearest neighbor hopping and so on, and to next nearest neighbor Coulomb interaction, as well as to multi orbital physics. The corresponding phase diagram becomes more complicated. Here we only focus on the single-band case as in eq (2).

- Pictorically:



→ The first term gives the quantum tunneling between nearest sites, obtained by the kinetic energy and ionic potential energy as we have seen in the tight binding model. For $t>0$, the energy is gained for an electron to tunnel to the nearest site, and hence metalicity is favored. Note that in this quantum tunneling, often called electron hopping, the spin is conserved, so this is not directly blocked by the Hubbard U.

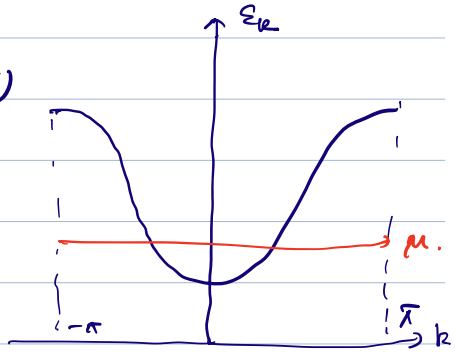
→ The chemical potential term says for $\mu>0$, energy is gained for an electron to stay at its site. Therefore, it's a competition between μ & t which governs a metal to "band insulator" behavior. This can be easily seen by going to the momentum space, where the first term becomes diagonal: For $U \to 0$, we have

$$H = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k\sigma} c_{k\sigma}. \qquad -- (3a)$$

where $$\varepsilon_k = -2t(\cos k_x + \cos k_y + \cos k_z) - \mu \qquad -- (3b)$$

in a 3D square lattice (the result depends on lattice structure). The band bottom occurs at $k=(0,0)$ with energy $-6t$ and top at $k=\pm(\pi,\pi)$ with energy $+6t$. Therefore, the metallic behavior occurs for.

$$-6t \le \mu \le 6t. \quad , \mu>0, t>0.$$



→ Now we turn on $U \gtrless 0$. U is only effective at a site if the site is already occupied, otherwise $n_{i\sigma} = 0$. And since $U > 0$, so it increases the energy by U to have two particles at the same site, and hence its disfavored. But adding 2-particles at a given site decreases energy by -2μ, giving a total energy of $-2\mu + U$. On the other hand, if the two particles are in in any two different sites we gain energy by $-2\mu < -2\mu + U$, so, they will not like to be at the same site.

There are two scenarios when the situation becomes complicated: For $t > 0$ and at greater than half-filling fraction.

Suppose two electrons are sitting in two adjacent sites. If they sit on two different sites we gain energy by -2μ. But if one electron tunnels to the adjacent site, we have an energy $-2\mu - t + U$.* Now, the situation depends on whether $U > t$ or $U < t$. For $U > t$, we electron will not hop, and we have an insulator - called the Mott insulator. At $U < t$, the electron will hop to lower the energy - so we have a metal. $U = t$ marks hence the metal-insulator phase transition point.

But the phase diagram also depends on another factor - the number of electrons - called the filling fraction. Lets start with $N = 2$-site problem, which has $2^N = 4$ states. We give M electrons (with 2-spin states), with $0 \leq M \leq 2$, then the filling fraction $n = M/N$, which ranges from $0 \leq n \leq 2$, including the spin. (Sometimes you have to be careful if the reported value of n includes the spin (and orbital / sublattice) states also or not.)

(* For $t \neq 0$, the occupation number n_i at a site is not a conserved quantity and hence the exact value of n_i at a site cannot be defined. See below).

- For $M=0$, $n=0$: $E=0$.
- For $M=1$, $n=1/2$: $E=-\mu$, with 4-fold degeneracy:
  $\uparrow -$, $\downarrow -$, $-\uparrow$, $-\downarrow$.

  This is clearly a Band metal.
- For $M=2$, $n=1$:

$|\psi_1\rangle$: $\uparrow\uparrow$, $\downarrow\downarrow$, $E_1=-2\mu$, Ferromagnet
$|\psi_2\rangle$: $\downarrow\uparrow$, $\uparrow\downarrow$, $E_1=-2\mu$, Spin density wave / Antiferromagnet
$|\psi_3\rangle$: $\uparrow\downarrow -$, $-\uparrow\downarrow$, $E_2=-2\mu+U$, Charge density wave.

→ The first case is a Ferromagnet. In the second one, the spins are staggered and hence it's a spin density wave (SDW) or antiferromagnetic case. Both FM & AFM have the same energy. In the large-N system this degeneracy is lost and one often gets an AFM at half-filling ($n=1$). The last one has 2-electrons at one site and one empty site. Since the # of electrons are different in adjacent sites, so, the charge density is different at different site. This is called the charge density wave (CDW) state. Both CDW & SDW breaks the lattice translational symmetry, and the unit cell is now doubled - now containing two sublattices.

As we turn on $t \neq 0$ term, this Hamiltonian does <u>not</u> commute with the local density operator $n_{i\sigma}$, and none of the above states are the eigenstates of H. This is because t term allows to hop an electron from one site to

another. In the FM case, the Pauli exclusion principle blocks the electrons to hop between the same spin sites. In the SDW state, the electron can hop to the other site and gain an energy $-t$, but have to overcome the onsite repulsion of U. In fact in this 2-site model, SDW & CDW states are not the eigenstates, and one can obtain an eigenstate by diagonalizing the Hamiltonian.

- $M=3,\ n=\frac{3}{2}$: $\uparrow\downarrow\ \uparrow$, $\uparrow\uparrow\ \downarrow$

  $E = -3\mu - t + U$:

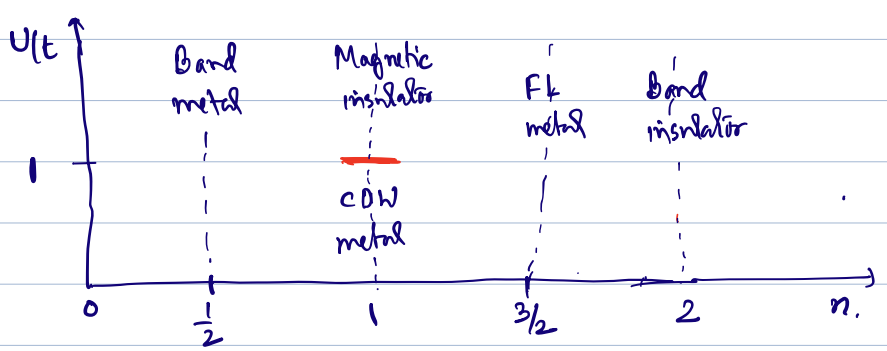
  This is a Fermi Liquid (metal).

- $M=4,\ n=2$: $\uparrow\downarrow\ \uparrow\downarrow$: $E = -4\mu$.

  Band insulator.

Therefore, the Quantum Phase diagram in terms of n & U/t.

(For 2-sites)



(*) $N \to \infty$ limit: Phases can look very different in real materials having $N \sim 10^{23}$. In this case the Hilbert space dimension is 2^N - which is exponentially large, and we cannot solve such a Hamiltonian exactly, because $2^N \times 2^N$-dimensional matrix cannot be diagonalized with any computer. (Presently $N = 10$-20 site lattice can be diagonalized exactly).

- In 1D Hubbard model is solved exactly, using the so-called Bethe Ansatz. In this approach, one maps the lattice to another lattice without any periodic boundary condition such that there arises N (or more) conserved quantities - i.e., operators which commute with the Hamiltonian. The eigenstates of these quantities are also the eigenstates of the Hamiltonian and thereby we get an idea about the energies.

→ In higher dimensions, the Hubbard model cannot be solved exactly. We can however obtain a few qualitative features as a function of $n = N/V$, can now take any fractional value between $0 \leq n \leq 2$. (In the thermodynamic limit of $N \to \infty$, $V \to \infty$ $n \to$ remains finite). The electron density n is directly related to the chemical potential, and hence the discussion with respect to n is equivalent to discussion with respect to μ.

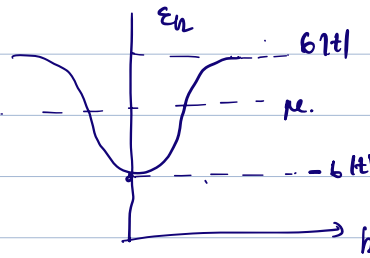
→ Similar qualitative behavior can also be deduced as a function of U/t, at least in the limits of $U/t \to 0$ & ∞.

In the limits of $U/t = 0$ & $U/t \to \infty$, the Hubbard model is exactly solvable. Because in these two limits there are extensive number of conserved quantities - which are the occupation density in the momentum & real space, respectively.

- At $U/t \to 0$: the Hamiltonian becomes.

$$H = -t \sum_{\langle ij \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} - \mu \sum_{i\sigma} n_{i\sigma}.$$

Here the local density operator $n_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ does not commute with H, but the momentum density operator $n_{k\sigma} = c_{k\sigma}^{\dagger} c_{k\sigma}$, commutes with H. Because, H is diagonal in the momentum space, and we have a band dispersion ε_k. $n_k = 0, 1$ is the corresponding $k > k_F$ or $k < k_F$. Therefore, this is a metal for $-6t \le \mu \le 6t$. In the language of filling fraction $n = \frac{1}{N} \sum_{k \le k_F} n_k$, the system is a metal for $0 \le n \le 2$.



- At $U/t = \infty$, ie, $t = 0$, we have

$$H = -\mu \sum_{i\sigma} n_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}.$$

$$= \sum_{i\sigma} h_{i\sigma}$$

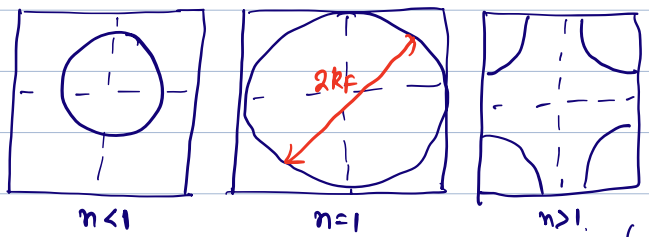
Here $[n_{i\sigma}, H] = 0$, but $[n_{k\sigma}, H] \neq 0$. This is obvious, the Hamiltonian is completely local, and only a potential energy is present. So, position is fixed. The energy levels are completely flat in the momentum space. So, it's an insulator at all filling factor n, but the type of insulating state varies with n.

→ For $n < 1$, ie, when the number of electron is less than the number of sites. All the sites will be either singly occupied or empty, because double occupancy costs $U \to \infty$ energy.

→ Ground state energy $E_0 = \sum_{k \le k_F} \varepsilon_k n_k$.

→ Excited states are putting electrons above the Fermi-level - creating one particle-hole excitations. One has a continuum of excitations - called the particle hole excitations.

- $n = 1$ (when $\mu = 0$) is however special. Here the Fermi surface is the largest as it encloses half of the Brillouin Zone. So, the Fermi surface touches the Brillouin zone boundary.



For $n < 1$, the Fermi surface was electron-like centering $k = (0, 0, 0)$ point, and for $n > 1$, the Fermi surface is hole like centring the BZ corner. So, at $n = 1$, the Fermi surface undergoes a topological phase transition - called the Lifshitz transition. (*) Here the sign of the charge density at the Fermi level (called

The ground state energy density is $E_0 = -\mu n$, and its first excited state is obtained by putting two electron in one site. So, $E_1 = -\mu(n V - 1) + U$. Since $U \to \infty$, so it an insulator. Its generally a Wigner crystal at low density, but it can have well defined lattice structure at commensurate filling factor, ie, when the number of site is some integer integer multiple of the number of electron. Then one would have some charge density wave or checkerboard structure. e.g. At $n = 1/2$, we have every alternative site one empty.

or At $n = 1/4$:

- $n = 1$. In this case we have exactly one electron per site. Clearly, the system can still avoid double

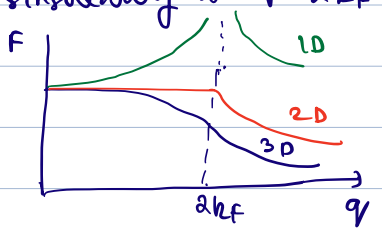
occupancy at any site.

This is still a Wigner crystal, with energy density $E = -t/2$.

Each site is spin degenerate. Since $t=0$, there is no coupling between sites and one cannot say anything about one site's state influence the nearest site and produce long-range / short range order.

the carrier density) changes from positive to negative, as one can measure from the Hall effect measurement.

Moreover, recall that in the Lindhard susceptibility $\chi(q,0) \to d(v)\, f(q/2k_F)$, and $f(q/2k_F)$ has a singularity at $q = 2k_F$

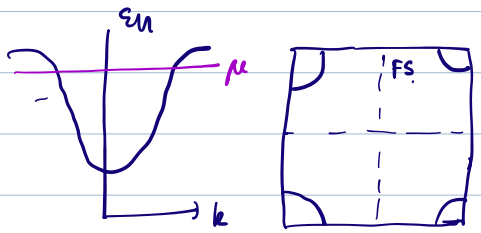


This singularity is now at $q = 2k_F = G/2$, ie, at half of the Brillouin zone. So, the system has the tendency to reduce the reciprocal lattice wave vector to half, ie, increase the lattice constant by 2. This is called the Fermisurface Nesting instability. (With little bit of interaction, this instability gives a singularity in the RPA susceptibility and the system tends to break the translational symmetry to a doubled unit cell with

two sublattices / basis-giving AFM phase.)

⊗ Disclaimer: Actually, the Lifshitz transition occurs slightly away from the $n=1$ value, at $\mu = -2t$ when $\epsilon_k = 0$ at $k = (\pi, 0), (0, \pi)$ and its equivalent points.

- $1 \ll n < 2$: In this case, the chemical potential lies near the band top, and the carrier density (i.e., the hole density) is small. This situation is now similar to the $n \ll 1$ case but now for holes. So, one gets a hole liquid, rather than an electron liquid.



- $1 < n < 2$: Now double occupance is inevitable in some sites and the ground state energy density is $E = -\mu/2 + U(n - \frac{1}{2})$.

e.g. At $n = 3/2$, we have

$\cdots \uparrow\downarrow \uparrow \uparrow\downarrow \uparrow \uparrow\downarrow \uparrow \cdots$

So, we will have a CDW insulator.

- $n = 2$: All sites are doubly occupied and the ground state energy is $-n\mu + nU$.

(*) Now we turn on the other term in the Hamiltonian. How are we going to approach the problem?

- Here we now introduce $U>0$, but $U/t \ll 1$ is small.

  n_k does not commute with the Hubbard interaction term. So, we cannot solve this Hamiltonian exactly. Here we can treat the interaction term perturbatively. The first order perturbation term is computed within the Hartree-Fock or Fermi-liquid approach – both are equivalent here.

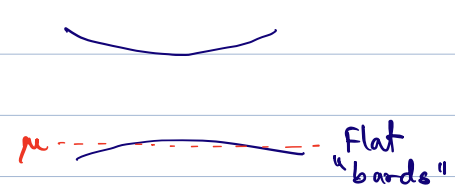
- $n \ll 1$: In the Hartree-Fock method, at low-density $n \ll 1$, the chemical potential is close to the bottom of the band, and we can almost approximate system as electron liquid with plane wave like solution. Because, the band bottom is near $k \sim 0$, with parabolic dispersion. So, here small k, i.e. large wavelength states

- Here we turn on $t>0$ and look at $t/U \gg 1$ limit perturbatively.

  n_i does not commute with the hopping term of the Hamiltonian, and a completely localized picture of $n_i = 0$ or 1 breaks down. Naturally, we will treat this problem perturbatively with the Hopping term being the perturbation. We can also do a mean field treatment by considering fluctuations around some mean values of n_i as

$$n_i \to \langle n_i \rangle + \delta n_i.$$

Not so much phase transition etc we find here except near half-filling ($n=1$), except that the localized energy levels of the $U \to \infty$ case now become dispersive and we get band with very narrow band width of $12t \ll U$.



If the chemical potential is

contribute, and for such long-wavelength states, the lattice constant, $a << \lambda$, is negligible. Therefore, these electrons behave like electron liquid. In the HF approach we will have direct, exchange, higher order corrections, but also need to consider screening. We will always get metallic state here, unless we increase U. Then r_s increases and we go towards the Wigner crystal region. But in between, one has interesting phase transition, that can not be predicted by the H-F theory. One needs to look at the time-dependent HF/ RPA theory or the Fermi-liquid approach or a mean field theory to predict some instability / singularity in the theory. For example, for the mean field theory, we will start with some average momentum density and consider its fluctuation

$$n_k \to \langle n_k \rangle + \delta n_k .$$

We can look at if there is any excited state defined by

turned inside such flat bands, we get a narrow region of what is called "correlated metals" such as CDW, FM or AFM metal as appropriate.

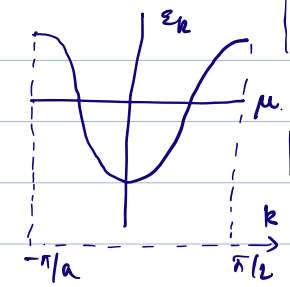
δn_k can become the ground state and hence one has a phase transition.

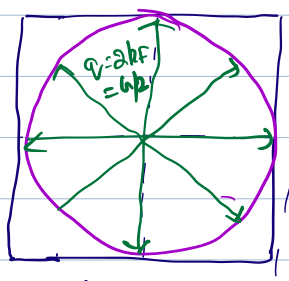
Equivalently, in the Fermi-liquid theory, we allow δn_k electrons to move past the Fermi-level due to interaction, and compute the self energy, renormalization factor Z, ie, the Landau parameter. So, in this description, the electron liquid is a Fermi liquid.

But the Fermi liquid description is valid till the renormalization $Z \to 0$, ie, $F_0^{(A,S)} = |d(0)\, f_0^{(A,S)}| \to 1$. For the Hubbard model, $f_0 \equiv U$ and $d(0)$. So, one hits an instability as $dU \to 1$, which occurs at higher U and/or with higher d. This is called the Stoner instability. The same result is also obtained through the RPA method as we will discuss in this course. Above this value of $dU \gtrsim 1$, one has a phase transition to FM or AFM phase depending,

on the details of the band structure and Fermi surface topology.

- **$n=1$** : This is actually a very unique situation and one has two phase transitions competing with each other. At this half-filling, the Fermi level lies at the middle of the band, and the Fermi surface encloses half of the Brillouin zone, because half of all the k-points is now filled.





We have a Lifshitz transition at $U=0$, which now turns into a Stoner like instability but at finite $q = 2k_F = G/2$. in the RPA susceptibility. The instability is to be defined similarly as

$$1 - U\chi(q,0) = 0$$

$$\Rightarrow \boxed{U\, d(U)\, f(G/2k_F) = 0.}$$

- **$n=1$**: Interesting features are also expected near half-filling in the $t/U \gg 1$ limit. We start with putting one electron at each site, with one hole/empty state for opposite spin. Each site is spin degenerate, which can now be broken by the introduction of t. In fact, we get an AFM state - which is called Mott antiferromagnet. This can be understood qualitatively as follows.

Once we put an electron at a site with say $\uparrow$-spin, then another electron with $\downarrow$-spin can be added at this site, but it costs $U \to \infty$ energy. The electron in the adjacent site will be $\downarrow$-spin, such that the total magnetization of the system is minimized (zero for an AFM). Therefore, an AFM ordering will be energetically favored than an FM order

$\cdots \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \cdots$

This instability arises in the spin density wave channel (to be discussed) and gives rise to an AFM phase.

(One sees such a phase in Cr-element, Cu based, iron based superconductors, and in several other examples.)

In the AFM phase, the electronic dispersion has a gap (we will see that in a Mean field theory) and with increasing U, the gap increases and one can get a phase transition / crossover from the AFM metal to AFM insulator.

Quantitatively, an AFM state is also understood by an effective model proposed by Anderson, called t-J model.

At $n=1$, and $U \to \infty$, we have two degenerate states at each sites: $|\uparrow\rangle$ & $|\downarrow\rangle$ which is gapped from $|\uparrow\downarrow\rangle, |0\rangle$ states by $U \to \infty$ energy. This two states can be thought of as the two states of a $S=1/2$ spin. In fact using degenerate perturbation theory, and treating the hopping Hamiltonian as perturbation, one obtains a Heisenberg Hamiltonian as

$$H \approx J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma}.$$

where $J = 4t^2/U > 0$. Since $J > 0$ the system lowers its energy by having the nearest spins antiparallel to each other. This model is slightly different from the Heisenberg spin model due to the presence of the electron hopping term. This is called the t-J model.

The t-term is only valid if there are holes in the system, i.e., in the neighborhood of $n < 1$. Because, an electron cannot hop to an singly

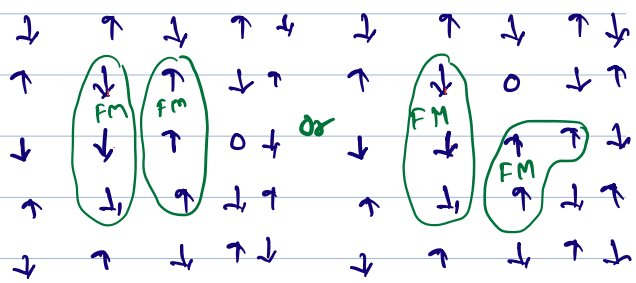
- $1 << n < 2$: In this case again, we start with a small but hole like Fermi surface, and turn on interaction adiabatically so, we will obtain a Fermi-hole liquid phase.

occupied site due to large U penalty. But an electron can hop to an adjacent site if its completely empty. So, the hopping is restricted here. An antiferromagnetic metallic phase arises eventually with $n < 1$, and with increasing t.

A similar AFM metal phase also arises in this region of $U/t \sim 1$, if we start from the band picture, as described in the L.H.S. This is to say that in this $U/t \sim 1$ region, there is no clear starting ground state and a small perturbation parameter. This region is generally very challenging to model both analytically as well as numerically.

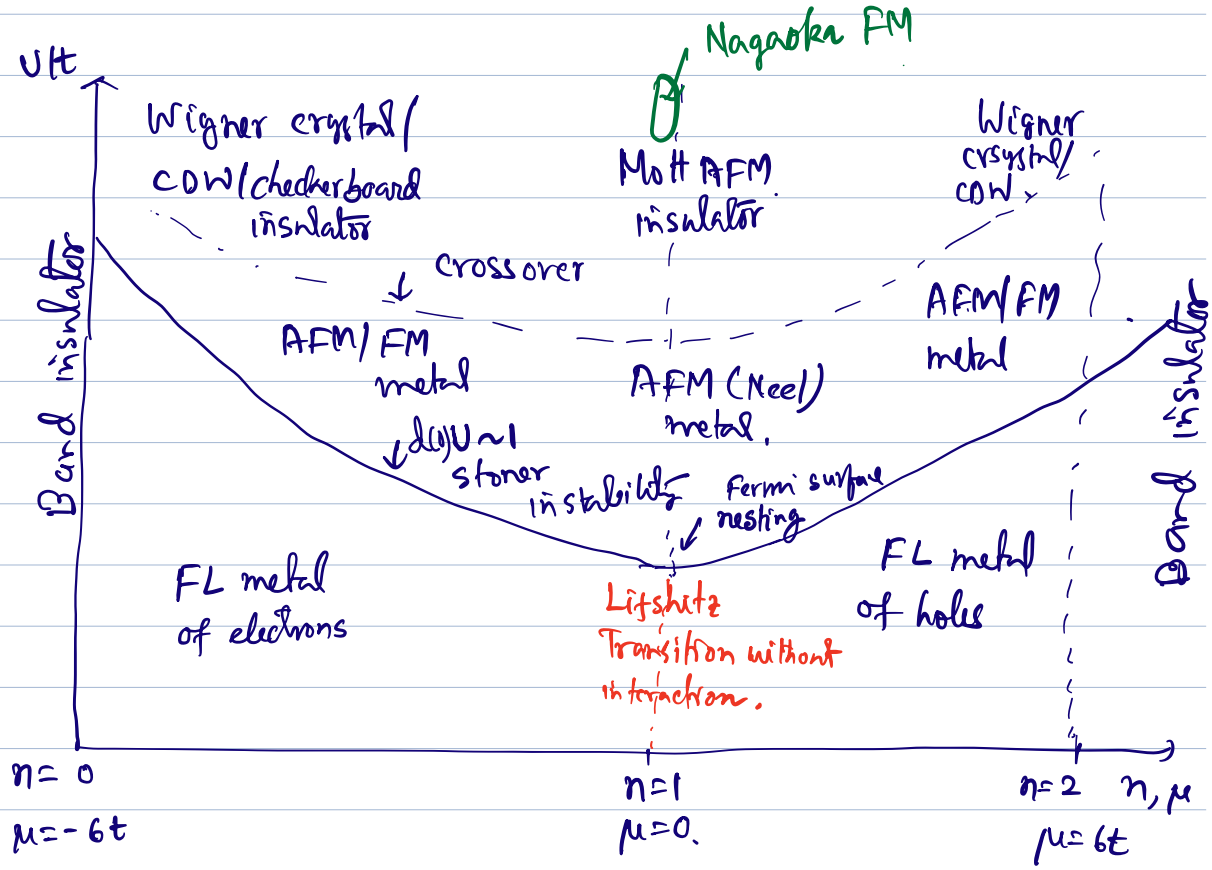
→ $n \sim 1$ but $n < 1$.

In this limit of very few holes in the lattice and $U/t \gg 1$, there exists an interesting phase – called the Nagaoka Ferromagnet. This can be qualitatively understood as follows. Imagine we start with an AFM insulator at $n=1$ and add a single hole.



We observe that everytime the hole moves it creates a domain of FM. None of these states are the eigenstates, and so one takes a linear combination of all such spin configurations. Then it can be shown that the final result is a FM, in which the hole can move freely. This gives a flat band Ferromagnet

- Taken together, the qualitative phase diagram of the Hubbard model is as follows.



(#) Symmetries of the Hubbard Model.

The Hubbard model has several symmetries hidden in its form, and hence breaking of those symmetries to form new quantum phases of matter.

- Translational symmetry: Because the Hubbard interaction is present at all lattice sites, so translational symmetries of the lattice are all preserved in this model.

- Spin rotational symmetry: $\vec{S} \to -\vec{S}$. (Spin inversion symmetry $S_x \to S_y$, $S_y \to S_z$, $S_z \to S_x$ Rotational symmetry)

→ As we know the spin at a site is denoted by

$$\vec{S}_i = \frac{1}{2} c^\dagger_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta} \quad \text{--- (3a)}$$

which gives

$$S^x_i = \frac{1}{2} c^\dagger_{i\uparrow} c_{i\downarrow} + c^\dagger_{i\downarrow} c_{i\uparrow} \quad \text{(3b)}$$

$$S^y_i = \frac{1}{2} (c^\dagger_{i\downarrow} c_{i\uparrow} - c^\dagger_{i\uparrow} c_{i\downarrow}) \quad \text{(3c)}$$

$$S^z_i = \frac{1}{2} (c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}) \quad \text{(3d)}$$

$$= \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow})$$

$$S^\pm_i = S^x_i \pm i S^y_i = c^\dagger_{i\uparrow} c_{i\downarrow}, \; c^\dagger_{i\downarrow} c_{i\uparrow} \quad \text{(3e)}$$

[we set $\mu_B = 1$, $\hbar = 1$].

→ $$n_{i\uparrow} c_{i\downarrow} = c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow} = c^\dagger_{i\uparrow} c_{i\uparrow} (1 - c_{i\downarrow} c^\dagger_{i\downarrow})$$

$$= c^\dagger_{i\uparrow} c_{i\uparrow} + c^\dagger_{i\uparrow} c_{i\downarrow} c_{i\downarrow} c^\dagger_{i\uparrow}$$

$$= n_{i\uparrow} - c^\dagger_{i\uparrow} c_{i\downarrow} c^\dagger_{i\uparrow} c_{i\downarrow}$$

$$= n_{i\uparrow} - S^+_i S^-_i$$

Similarly we get $= n_{i\downarrow} - S^-_i S^+_i$

Now: $n_{i\uparrow} n_{i\downarrow} = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow}) - (S_i^{xx} + S_i^{yy})$ ---(a)

and $S_i^{zz} = \frac{1}{4}(n_{i\uparrow} - n_{i\downarrow})^2$

$= \frac{1}{4}\left[\underbrace{n_{i\uparrow}^2}_{= n_{i\uparrow}} + \underbrace{n_{i\downarrow}^2}_{n_{i\downarrow}} - (n_{i\uparrow} n_{i\downarrow} + n_{i\downarrow} n_{i\uparrow})\right]$.

$= \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2} n_{i\uparrow} n_{i\downarrow}$

$\Rightarrow \quad n_{i\uparrow} n_{i\downarrow} = \frac{1}{2}(\underbrace{n_{i\uparrow} + n_{i\downarrow}}_{n_{ic}}) - 2 S_i^{zz}$. ---(b)

n_{ic} = total number / charge density

Therefore, combining (a) & (b) we get

$$n_{i\uparrow} n_{i\downarrow} = \frac{1}{2} n_{ic} - \frac{2}{3} \vec{S}_i^{\,2} \quad \text{---(4)}.$$

This term is symmetric under the spin inversion and spin rotations.

- There are also particle-hole (electron-hole symmetry) of the Hubbard model on a 2-sublattice / bipartite lattice. (see P. Fazekas Page 171).

5.2 RPA theory of charge and spin susceptibility in the Hubbard model.

In Chapter 4, we studied only the density-density response function for a long-range Coulomb interaction. We found a new collective mode from the vanishing of the RPA denominator at high frequency - which is the Plasmon mode, and also two static properties - namely the Thomas-Fermi screening and Friedal oscillations - in which the electron density gets redistributed to screen a local charge fluctuations, but does not cause an instability or singularity.

Now we want to investigate this problem for a Hubbard interaction - mainly in the static limit. We will find instability in the spin density channel at $q=0$ and/or a similar instability at finite $q=Q$ value, signaling a ferromagnetic or antiferromagnetic (spin density wave) phase, respectively. This is generally called the Stoner instability or Fermi surface nesting instability, respectively.

At finite frequency also, we obtain similar collective excitations in the RPA channel for spin case - which is called the magnon mode.

- we want to compute the charge $\delta\rho_c(r) = \frac{1}{2}(\delta\rho_\uparrow + \delta\rho_\downarrow)$ and spin $\delta\rho_s(r) = \frac{1}{2}(\delta\rho_\uparrow - \delta\rho_\downarrow)$ density response functions, defined as

$$\chi_c(q,t) = -\frac{i}{\hbar}\theta(t)\langle[\delta\rho_c(q,t), \delta\rho_c(-q,0)]\rangle, \quad \text{--- (4a)}$$
$$\chi_s(q,t) = -\frac{i}{\hbar}\theta(t)\langle[\delta\rho_s(q,t), \delta\rho_s(-q,0)]\rangle, \quad \text{--- (4b)}$$

where $\delta\rho_\sigma(q,t) = \sum_k c^\dagger_{k+q,\sigma}(t)\, c_{k,\sigma}(t)$, $\sigma = \uparrow, \downarrow$

where the expectation value is computed for the non-interacting case first, and then for a time-dependent Hartree-Fock state (RPA) in a thermal ensemble.

Because of the non-interacting nature of the states in the expectation value, the Wicks theorem remains valid. Therefore, as we expand the commutators, and splits four-fermion operators into the expectation values of pair of fermions, only the same-spin density terms such as $\langle\delta\rho_\sigma\rangle$ survive, while spin flip terms such as $\langle c^\dagger_{k\uparrow} c_{k\downarrow}\rangle$ terms disappear. Therefore, only consider the density-operator terms and obtain:

$$\chi_{c,s}(q,t) = -\frac{i}{4\hbar}\theta(t)\langle[(\delta\rho_\uparrow \pm \delta\rho_\downarrow), (\delta\rho_\uparrow \pm \delta\rho_\downarrow)]\rangle, \quad (q, t \text{ dependences are implicit}).$$
$$= -\frac{i}{4\hbar}\theta(t)\langle[\delta\rho_\uparrow, \delta\rho_\uparrow] + [\delta\rho_\downarrow, \delta\rho_\downarrow] \pm [\delta\rho_\uparrow, \delta\rho_\downarrow] \pm [\delta\rho_\downarrow, \delta\rho_\uparrow]\rangle$$
$$= -\frac{i}{4\hbar}\theta(t)\sum_{\sigma\sigma'}\sigma\sigma'\langle[\delta\rho_\sigma, \delta\rho_{\sigma'}]\rangle, \quad \sigma, \sigma' = \pm 1 \text{ for } \uparrow, \downarrow.$$

$$= \sum_{\sigma\sigma'}\sigma\sigma'\,\chi_{\sigma\sigma'}(q,t). \quad \text{-- (5a)}$$

- Now, $\chi_{\sigma\sigma'}(q,t) = -\frac{i}{4\hbar}\theta(t)\langle[S_\sigma(q,t), S_{\sigma'}(-q,0)]\rangle$

$$= -\frac{i}{4\hbar}\theta(t)\sum_{k,k'}\Big(\langle c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\, c^\dagger_{k'-q\sigma'}(0)\, c_{k'\sigma'}(0)\rangle - \langle c^\dagger_{k'-q\sigma'}(0)\, c_{k'\sigma'}(0)\, c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\rangle\Big)$$

$$\langle c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\, c^\dagger_{k'-q\sigma'}(0)\, c_{k'\sigma'}(0)\rangle$$

$$= \langle c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\rangle\langle c^\dagger_{k'-q\sigma'}(0)\, c_{k'\sigma'}(0)\rangle + \langle c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\,(\delta_{k',k'-q} - c_{k'\sigma'}(0)\, c^\dagger_{k'-q\sigma'}(0))\rangle$$

$$= \text{same} + \langle n_{k\sigma}(t)\rangle\delta_{q,0} + \langle c^\dagger_{k+q}(t)\, c_{k'\sigma'}(0)\, c_{k\sigma}(t)\, c^\dagger_{k'-q\sigma'}(0)\rangle$$

$$= \text{same} + \text{same} + \langle c^\dagger_{k+q\sigma}(t)\, c_{k'\sigma'}(0)\,(\delta_{k,k'-q}\delta_{\sigma\sigma'}\delta(t-0) - c^\dagger_{k'-q\sigma'}(0)\, c_{k\sigma}(t))\rangle$$

$$= \text{same} + \text{same} + \delta_{kk'}\delta_{\sigma\sigma'}\langle n_{k+q,\sigma}(0)\rangle - \langle c^\dagger_{k+q\sigma}(t)\, c_{k'\sigma'}(0)\rangle\langle c^\dagger_{k'-q\sigma'}(0)\, c_{k\sigma}(t)\rangle$$

similarly,

$\langle c^\dagger_{k'-q\sigma'}(0)\, c_{k'\sigma'}(0)\, c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\rangle$: we do the same anticommutation in the first two operators $(\delta_{k'k'-q} - c_{k'\sigma'}(0)\, c^\dagger_{k'-q\sigma'}(0))$ and then follow similarly. Then we get

$$= \langle c^\dagger_{k'-q'\sigma}(0)\, c_{k'\sigma'}(0)\rangle\langle c^\dagger_{k+q\sigma}(t)\, c_{k\sigma}(t)\rangle + \langle n_{k\sigma}(t)\rangle\delta_{q,0}\delta_{kk'}\delta_{\sigma\sigma'}\langle n_{k\sigma}(0)\rangle - \langle c^\dagger_{k'-q\sigma'}(0)\, c_{k\sigma}(t)\rangle\langle c^\dagger_{k+q\sigma}(t)\, c_{k'\sigma'}(0)\rangle$$

Then as we take the difference between the two terms, we find the first and last terms identically cancel each other. The 2nd term $\langle n_{k\sigma}(t)\rangle$ also gets cancelled. Finally we are left with

$$\chi_{\sigma\sigma'}(q,t) = -\frac{i}{4\hbar}\theta(t)\sum_{kk'}\delta_{\sigma\sigma'}\delta_{kk'}\left(\langle n_{k\sigma}(0)\rangle - \langle n_{k+q\sigma}(0)\rangle\right) \quad --(5b)$$

Remarkably, this is exactly the same form we obtained in the

chapter 4 for the density response function for each spin. Therefore, we substitute eq (56) in (54) and obtain:

$$\chi_{c,s}(q,t) = -\frac{i}{2\hbar}\theta(t)\sum_{k}\left[\underbrace{\langle n_{k\sigma}(0)\rangle}_{f(\varepsilon_{k,\sigma})} - \underbrace{\langle n_{k+q,\sigma}(0)\rangle}_{f(\varepsilon_{k+q,\sigma})}\right].$$

In the frequency space we get

$$\boxed{\chi_{c,s}(q,t) = \frac{1}{2V}\sum_{k,\sigma}\frac{f(\varepsilon_{k,\sigma}) - f(\varepsilon_{k+q,\sigma})}{\omega + \varepsilon_{k\sigma} - \varepsilon_{k+q,\sigma} + i\eta}} \quad \text{—(6)}$$

So, the spin and charge fluctuates in the same way for a non-interacting and spin unpolarised case. Therefore, the physics of the particle-hole excitations is the same.

The spin and charge susceptibilities become decoupled in the RPA channel.

⊛ RPA theory of the Hubbard model:

Recall that RPA theory is nothing but a time-dependent mean-field theory. For the charge and spin density response, we employ the mean value of the charge & spin densities, respectively. Hence it's convenient to express the Hubbard model in terms of these densities.

Recall that: $\rho_{i\uparrow} = \rho_{ic} + \rho_{is}$, $\rho_{i\downarrow} = \rho_{ic} - \rho_{is}$, where ρ_{ic}, ρ_{is} are the charge, spin densities at the i^{th} site. So, we get

$$H_U = U\sum_i (\rho_{i\uparrow}\rho_{i\downarrow} + \text{h.c.}) = \frac{U}{2}\sum_i (\rho_{ic}\rho_{ic} - \rho_{is}\rho_{is})$$
$$= \frac{U}{2V}\sum_q \left[\rho_c(q)\rho_c(-q) - \rho_s(q)\rho_s(-q)\right] \quad -(7).$$

→ For the charge case, we add an external perturbation

$$H'(t) = \frac{1}{2V}\sum_q \phi_{ext}(q,t)\,\rho_c(-q). \quad -(8a)$$

In this case, the time-dependent mean-field expansion of the charge as

$$\hat{\rho}_c(q) = \langle \rho_{c,ind}(q,t)\rangle + \hat{\rho}_c(q)$$

number (mean value) ↝ operator (fluctuations).

and $\langle \rho_s \rangle = 0$.

Thus,

$$H_U = \frac{U}{2V}\sum_q \rho_{c,ind}(q,t)\,\hat{\rho}_c(-q) \quad -(8b).$$

Thus $H_U + H'(t) = \tilde{H}'(t) = \frac{1}{2V}\sum_q \phi_{tot}(q,t)\,\hat{\rho}_c(-q)$ - (8c)

where $\phi_{tot}(q,t) = \phi_{ext}(q,t) + U\,\delta_{c,ind}(q,t)$ — (8d)

- Then according to the Linear response theory

$$\delta_{c,ind}(q,\omega) = \chi_c(q,\omega)\,\phi_{tot}(q,\omega). \quad \text{-- (8e)}$$

and $\delta_{c,ind}(q,\omega) = \chi_c^{RPA}(q,\omega)\,\phi_{ext}(q,\omega)$ --(8f)

So, substituting eq (8e) in eq (8d), we get

$$\phi_{tot} = \phi_{ext} + U\chi_c\,\phi_{tot}$$

or, $\phi_{tot} = \phi_{ext}/(1 - U\chi_c)$ -- (8g)

And substituting eq (8g) in eq (8e), we get

$$\boxed{\chi_c^{RPA}(q,\omega) = \frac{\chi_c(q,\omega)}{1 - U\chi_c(q,\omega)}} \quad -(8h).$$

- At $q \to 0, \omega \to 0$, we have $\chi_c(q,\omega) = -d(0)$. Hence the RPA denominator $1 + d(0)U$ does not vanish for any value of $U > 0$. Hence there is no singularity in the theory at $q \to 0$.

- At $\omega \to 0$, $\chi_c(q,\omega) = -d(0)\,f(q/2k_F)$. Since $f > 0$, so, there is no singularity at finite value of q as well.

- At $\omega \to \infty$ $(\omega >> v_F q)$ $\chi_c(q,\omega) = \frac{nq^2}{m\omega^2}$.

Then $\chi_c^{RPA}(q,\omega) = \frac{nq^2/m\omega^2}{1 - \frac{nq^2}{m\omega^2}U} = \frac{nq^2}{m}\,\frac{1}{\omega^2 - \omega_c^2(q)}$.

where $\omega_c^2(q) = nUq^2/m$ is a collective mode. For charge susceptibility, one needs to also include the long-range Coulomb interaction.

→ Next we consider the spin part. Similarly, we employ time-dependent mean-field theory for spin as

$$\delta_S(q) = \underbrace{\delta_{S,\text{ind}}(q,t)}_{S_z(q,t)} - \hat{\delta}_S(q) \quad \text{--- (9g)}$$

$[\mu_B = 1]$.

Then from the Hubbard model we get

$$H_U = \frac{U}{2V} \sum_q S_z(q,t)\, \delta_S(-q) \quad \text{--- (9b)}$$

Again for the calculation of the spin susceptibility, we add an external magnetic field along the z direction, which gives a perturbation term as

$$H'(t) = -\frac{1}{2V} \sum_q B_{ext}(q,t) \underbrace{S_z(-q)}_{\delta_S(-q)} \quad \text{--- (9c)} \quad [m_z = \mu S_z = S].$$

Then we get $H_U + H'(t) = -\frac{1}{2V} \sum_q B_{tot}(q,t)\, \delta_S(-q)$ --- (9d)

where $B_{tot}(q,t) = B_{ext}(q,t) - U S_z(q,t)$. --- (9e).

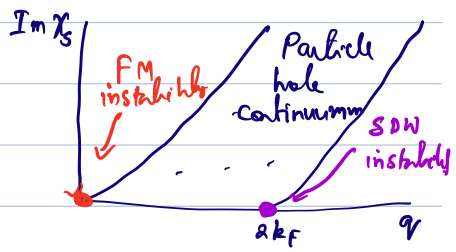
Then using the linear response theory, we get

$$\begin{aligned} S_z(q,w) &= \chi_s(q,w)\, B_{tot}(q,w) \\ &= \chi_s^{RPA}(q,w)\, B_{ext}(q,w). \end{aligned}$$

Proceeding similarly, we get

$$\boxed{\chi_s^{RPA}(q,w) = \frac{\chi_s(q,w)}{1 + U\,\chi_s(q,w)}} \quad -(9h).$$

Now, because of the opposite sign in the RPA denominator for spin, we get new singularity at $\omega \to 0$, when the RPA denominator diverges at $q = 0$ & at $q = 2k_F$, respectively FM & SDW states appear.



(a) Stoner instability We know that $\chi_0(q \to 0, \omega \to 0) \to -d(0)$

So, the RPA susceptibility diverges when the denominator vanishes

i.e., $$\boxed{U\, d(0) = 1} \qquad -- (10a)$$

or, $$U_{crit} = 1/d(0) \qquad -- (10b)$$

At this critical value of $U = \frac{1}{d(0)}$, the interacting or total spin response function diverges, i.e, becomes singular. This suggests that at this point the entire spin density will deform into some rearrangement of spin density to avoid this singular behavior. This is to say there is a phase transition from spin degenerate ground state to some ground state in which spin density is deformed into uniform ($q \to 0$) and static ($\omega \to 0$) value. Since spin density is defined as $(\rho_\uparrow - \rho_\downarrow)/2$, therefore, the spin up density will be higher than the spin down one at all positions (uniform). This is the Ferromagnetic phase.

(The physics is similar to Screening, but for spin density here. In the case of charge screening we had $\rho_{tot} = \rho_c^{ext} + \rho_c^{ind} = (1 + U\chi_c)\rho_{ext}$ $= \varepsilon^{-1}\rho_{ext}$, where the induced charge $U\chi_0\rho_{ext}$ screens the original charge density. Similarly here induced spin density is $\rho_s^{ind} = \rho_z^{ind} = -U\chi_0 S_z$ screens the original spin density of $S_z = \rho_s$. This leaves the system in a magnetized state permanently. Here

B_{ext} is like a test field, physically this means if there is an intrinsic spin fluctuation causing an intrinsically generated magnetic field, this leaves the entire system magnetized into a ferromagnetic ground state. This is the signature of a phase transition and the Stoner instability predicts a phase transition point.

(b) SDW instability at $q \neq 0$:

Now, we can look into some possible instability in the RPA susceptibility at finite momentum $q \neq 0$. Recall for the charge susceptibility case that the singularity in χ at $q = 2k_F$ gave a charge oscillation in real space at the wave vector $q = 2k_F$ - which is called the Friedal oscillation. In the present case we get a similar feature of spin density oscillation which we call the spin density wave order. A special case of the spin density wave is the Antiferromagnet when $q = G/2$, ie, half of the reciprocal lattice vector.

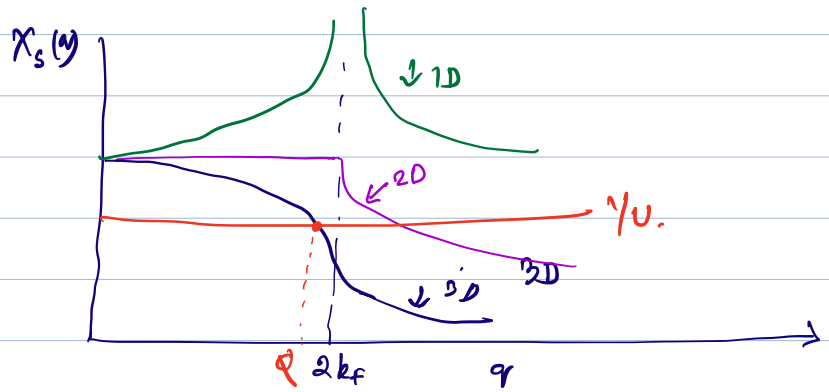
Since $\chi_s(q, 0) = -d(0)\, F(q/2k_F)$, we get from the spin RPA denominator $= 0$ condition satisfied at a partical value Q:

$$1 - U\, d(0)\, F(Q/2k_F) = 0 \qquad (11a)$$

$$\Rightarrow \quad d(0)\, F(Q/2k_F) = 1/U \,. \qquad (11b)$$

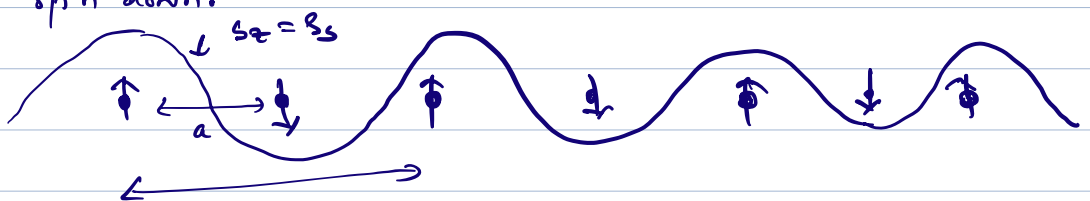
In such a case, a similar calculation as in the Friedal oscillation case, gives the spin density wave (oscillation) as

$$\boxed{S_z(r) = S_z(Q) \cos(Q \cdot r)} \quad \cdots \quad (12).$$



We see that for a given Fermi surface, $\chi_s(q) = 1/U$ condition can be satisfied for any value of U as long as it falls under the bandwidth of the material. Therefore, in principle, one has the SDW instability for any value of q for a given U. But if the corresponding q-value is not an rational number fraction of the reciprocal lattice vector, then the spin density wave has a very different lattice structure than the original lattice. It's called the incommensurate SDW. They tend to have very short life time and are often not very stable.

But for the case when $Q = G/2$ (or some rational number multiplication of of G), then then according to eqn (a), the spin density is repeated in twice the lattice constant of the original lattice, and at the original lattice site, it has the opposite phase, i.e. spin down.



This is the Antiferromagnetic phase. When $Q = 2k_F$, then the Fermi surface singularity is responsible for this SDW state and this is called the Fermi surface nesting instability.

5.3 Mean-field Theory of Ferromagnet:

Next we develop a static mean-field theory of the FM phase in the Hubbard model. This is to say in eq (9a), we assume the mean-spin density is static i.e.,

$$S_s(q) \equiv S_z(q) = \underbrace{\langle S_z(q=0, t=0)\rangle}_{\text{FM magnetization}} + \underbrace{S_z(q)\,\delta_{q=0}}_{\text{Magnetization fluctuation in also considered at } q=0 \text{ (uniform) as they turn out to be low-energy excitation (magnon) in a FM.}} \quad --(13)$$

We define the uniform magnetization

$$m = \langle S_z\rangle / V. \quad ---(14)$$

$$H_U = -U \sum_{q} S_s(q)\, S_s(-q)\, \delta_{q,0} + U \sum_{q} \underbrace{\langle S_c(q)\, S_c(-q)\rangle}_{n^2.}$$

$$= -U \sum_{q} \Big[\underbrace{\langle S_s(q)\rangle}_{m} S_s(-q) + \underbrace{\langle S_s(-q)\rangle}_{m} S_s(q) + \underbrace{\langle S_s(q)\rangle \langle S_s(q)\rangle}_{m^2.}\Big]\delta_{q,0} + U n^2$$

[c.f the mean-field expansion $S_1 S_2 = \langle S_1\rangle S_2 + \langle S_2\rangle S_1 - \langle S_1\rangle\langle S_2\rangle$

$$\approx -2Um\, S_s(0) - Um^2 + \underbrace{\theta(S_s^2)}_{\text{ignore since we are interested in small fluctuations}} + Un^2$$

$$= -\frac{2Um}{2} \sum_{k} \left(c^{\dagger}_{k\uparrow} c_{k\uparrow} - c^{\dagger}_{k\downarrow} c_{k\downarrow}\right) - U(m^2 - n^2) \quad --(15)$$

[we need the constant valued last term to show that the resultant total energy is lower than the non interacting theory above the Stoner criterion].

- Now plugging this mean-field valued H_0 in the total Hamiltonian we get the mean-field (MF) Hamiltonian as

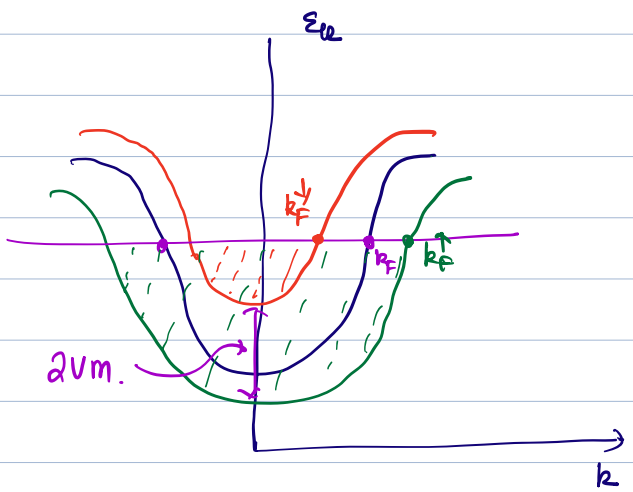
$$H_{MF} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} - Um \sum_k \left(c^\dagger_{k\uparrow} c_{k\uparrow} - c^\dagger_{k\downarrow} c_{k\downarrow} \right) - U(m^2 - n^2)$$

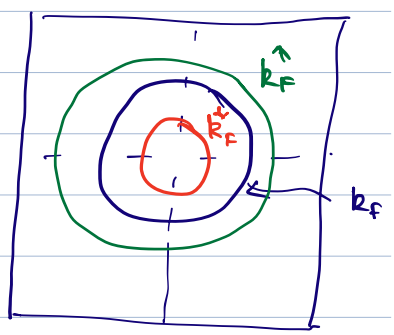
$$= \sum_{k,\sigma} \varepsilon^\sigma_k c^\dagger_{k\sigma} c_{k\sigma} - U(m^2 - n^2) \quad \text{---(16a)}$$

where $\varepsilon^\sigma_k = \varepsilon_k - \sigma Um$, where $\sigma = \pm 1$ for $\uparrow, \downarrow$.

---(16b)

Therefore, the non-interacting band structure now splits into up and down spin bands, with $2Um$ being the uniform (k-independent) gap between them. Because of this uniform gap structure for the ferromagnetic state, we can interpret it as the chemical potential is now different for the two spin states. In other words, now there are more up-spin states than the down spin states, and their corresponding Fermi surface volume are also different, to account for this difference.





Eq(16b) can also be interpreted as $\varepsilon_k^\sigma = \varepsilon_k + \Sigma_k^\sigma$, where $\Sigma_k^\sigma = -\sigma U m = U\langle S_\sigma \rangle$ = Hartree like Self energy term we defined in the Fermi liquid theory where $U \equiv f_0^{(A)}$ and $S_\sigma \equiv n$.

- The mean field wave function is

$$|\Psi_{MF}\rangle = \prod_{k \in k_F^\uparrow} c_{k\uparrow}^\dagger \prod_{k \in k_F^\downarrow} c_{k\downarrow}^\dagger |0\rangle \quad \cdots (17).$$

- Self-consistent ferromagnetic gap equation

(*) There is another way we can figure out these critical points in terms of U & T. Recall the definition of the magnetization in eqn (14)

$$m = \frac{1}{V} \langle S_s \rangle \qquad --(14)$$

where the expectation value of the spin density operator S_s is taken with respect to the mean-field wavefunction in eqn (17). The mean-field wavefunction depends on the magnetization as well (embedded in the value of $k_F^{\uparrow}$). Therefore, eqn (14) is a self-consistent equation for m. For a given value of U (and T) if there exists a solution of $m \neq 0$, then we have the FM phase, otherwise its a paramagnet ($m=0$), since $m=0$ is always a trivial solution

This can be calculated as follows:

$$m = \frac{1}{2V} \sum_k \left[\langle \Psi | c_{k\uparrow}^{\dagger} c_{k\uparrow} | \Psi \rangle - \langle \Psi | c_{k\downarrow}^{\dagger} c_{k\downarrow} | \Psi \rangle \right].$$

$$= \frac{1}{2V} \sum_k \left(f(\varepsilon_k^{\uparrow}) - f(\varepsilon_k^{\downarrow}) \right) \quad ; \quad \varepsilon_k^{\uparrow\downarrow} = \varepsilon_k \mp Um.$$

$$= \frac{1}{2V} \sum_k \frac{f(\varepsilon_k^{\uparrow}) - f(\varepsilon_k^{\downarrow})}{\varepsilon_k^{\uparrow} - \varepsilon_k^{\downarrow}} \times (2Um)$$

$$= -Um \; \chi(q=0, \omega=0)$$

$$\Rightarrow \quad \boxed{U \chi(0,0) = -1} \quad --(19a)$$

$$\text{or,} \quad \boxed{U d(0) = 1} \quad --(19b) \qquad \text{At } T=0.$$

This is exactly the Stoner criterion, which also turns out to be the self-consistent gap equation for the FM gap Δ_m or the self-consistent magnetization equation. Because the instability occurs at $q \to 0$, so the non-interacting band is fully gapped at all k-points. The FM ground state clearly has a lower energy by $2\Delta_m$ compared to the non-interacting one.

Thereby we get the same relation that $d(0)U = 1$ is the critical value of the interaction parameter for the theory to have a finite solution. To compute the value of Δ_m at a value of $U > 1/d(0)$ we need to go to the higher power terms of U on the R.H.S.

H.W. Calculate eq (16) at finite temperature and show that T_c is defined by

$$k_B T_c = \sqrt{\frac{U d(0) - 1}{\frac{\pi^2}{6} |d''(0)|}}$$

showing that $T_c = 0$ at $U d(0) = 1$ and $T_c > 0$ for $U d(0) > 1$.

- Next we can obtain the total energy of the MF theory as

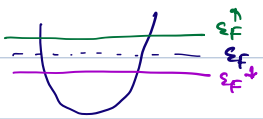
$$E_{MF} = \langle \Psi_{MF} | H_{MF} | \Psi_{MF} \rangle$$
$$= \sum_{k,\sigma} \varepsilon_k^\sigma \underbrace{\langle \Psi_{MF} | c_{k\sigma}^\dagger c_{k\sigma} | \Psi_{MF} \rangle}_{f(\varepsilon_k^\sigma) \text{ at some thermal equilibrium.}} - U(m^2 - n^2)$$
$$= \sum_{k,\sigma} \varepsilon_k^\sigma f(\varepsilon_k^\sigma) - U(m^2 - n^2)$$

$$\sum_k = \frac{V}{(2\pi)^3} \int d^3k = \int d\varepsilon\, d(\varepsilon)$$
dos

- $\sum_{k,\sigma} \varepsilon_k^\sigma f(\varepsilon_k^\sigma) = \sum_\sigma \int_{-\infty}^{\infty} d(\varepsilon_\sigma)\, \varepsilon_\sigma\, f(\varepsilon_\sigma)\, d\varepsilon$

As $T \to 0$:

$$= \sum_\sigma \int_{-\infty}^{\varepsilon_F^\sigma} d(\varepsilon_\sigma)\, \varepsilon_\sigma\, d\varepsilon, \qquad \text{where } \varepsilon_\sigma = \varepsilon + \sigma U m.$$



$$= 2\int_{-\infty}^{\varepsilon_F} \varepsilon\, d(\varepsilon)\, d\varepsilon + \sum_\sigma \int_{\varepsilon_F}^{\varepsilon_F - \sigma U m} d(\varepsilon)\, \varepsilon\, d\varepsilon$$

E_0 = non-magnetic ground state energy.

we often assume $d(\varepsilon) \approx d(0)$ as $d(\varepsilon)$ is weakly ε-dependent near ε_F.

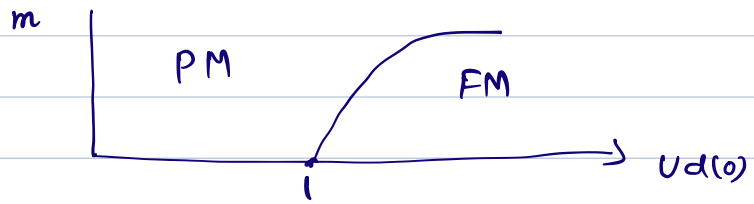
$$= E_0 + d(0) \sum_\sigma \varepsilon^2 \Big|_{\varepsilon_F}^{\varepsilon_F - \sigma U m}$$
$$= E_0 + \left[(\varepsilon_F - Um)^2 + (\varepsilon_F + Um)^2 - 2\varepsilon_F^2 \right] d(0)$$
$$= E_0 + 2\, d(0)\, (Um)^2$$

- Therefore, the mean field energy is

$$E_{MF} = E_0 + 2\, d(0)(Um)^2 - U(m^2 - n^2)$$
$$= E_0 + 2Um^2(U\, d(0) - 1) + Un^2. \qquad -(18)$$

First term is the ground state energy for $m = 0$ (non magnetic case). The second term gives a negative contribution when $U d(0) < 1$. This is precisely the Stoner criterion for ferromagnetism.

The 2nd term becomes vanishes at the critical point of $U\,d(0) = 1$, which is the Stoner criterion and for $U\,d(0) > 1$, the 2nd term becomes negative. This means, the energy is lowered in the FM state ($m \neq 0$). Therefore, we have a quantum phase transition from the paramagnetic state to a FM state at $Ud = 1$.



This is a very different phase transition than the usual phase transition we see in statistical physics which occurs due to thermal fluctuations. Above we saw a new phase transition which is called the quantum phase transition - driven by the quantum fluctuations. Here also interaction (U) is necessary, but not only the interaction, but also Pauli exclusion principle which is embedded in the finite density of states ($d(0)$) is also necessary. The Coulomb interaction in the spin density channel is the exchange term which is negative. Therefore, a finite spin density at a site ($n_{i\uparrow} > n_{i\downarrow}$) forces the spin density at other sites to be finite, which lowers the energy. The only energy it has to compete here is the kinetic energy term, which is restricted due to the exclusion principle. The scenario is very similar to the $r_s \sim 1$ critical point we discussed in the Hartree-Fock theory. As $d(0)$ is, the number of particles at the Fermi level increases, the interatomic distance $r_s \sim n^{-1}$ decreases. So, the electrons tend to be localized.

What about the phase transition with temparature ?. There is of course a phase transition of the usual type at the curie temperature T_c. Here the mechanism of the phase transition is different. With increasing temparature, the electrons are thermally excited and this increases disorder in the system, which destroys the magnetic order. The measure of the disorder is entropy. So, we need to calculate the entropy and compare with the internal energy $F = E - TS$. As the entropy term increases, one has a phase transition at $T_c = E/S$. Since here the magnetization 'm' is the order parameter, so, the entropy can be expressed in terms of the magnetization, as we did above for the internal energy. Thus, as the coefficient of the m^2 term becomes negative above a critical temparature, it destroys the magnetic order.

5.4 Mean-Field Theory of SDW (AFM).

Next we discuss the case where a spin density wave forms at finite wavevector Q due to the Stoner like criterion at $1 - U\chi(Q,0) = 0$. We will mainly focus on the $Q = (\pi, \pi)$ case where an antiferromagnetism (AFM) form.

As before, we will be considering a time-independent mean-field theory for a mean-field SDW order at $q = Q$:

$$S_s(q) \equiv S_z(q) = \langle S_z(Q, t=0) \rangle + S_z(Q) \qquad --(20)$$

Here the magnetization order parameter is

$$m = \langle S_z(Q) \rangle$$

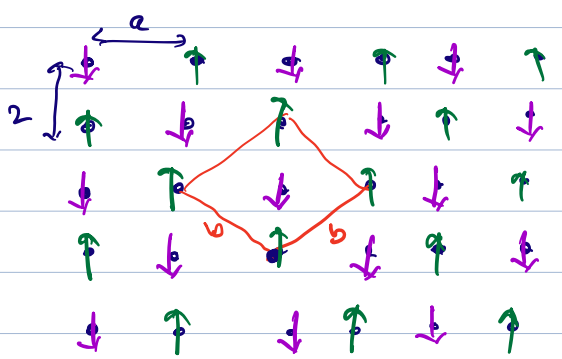
$$= \frac{1}{2} \sum_k \left[c^+_{k+Q\uparrow} c_{k\uparrow} \rangle - \langle c^+_{k+Q\downarrow} c_{k\downarrow} \rangle \right] ; \quad [\mu_B = \hbar = 1] \qquad --(21a)$$

$$= \frac{1}{2} \sum_{ij} \sigma \, c^+_{i\sigma} c_{j\sigma} e^{iQ(r_i - r_j)} \qquad --(21b)$$

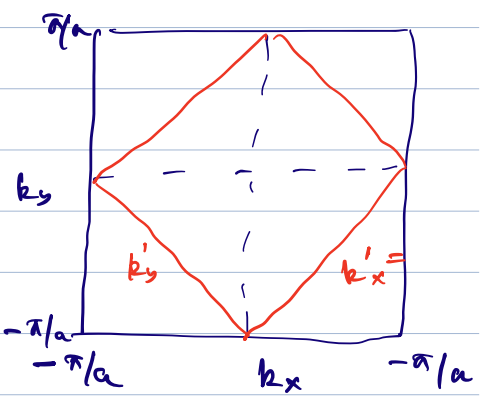
, $\sigma = \pm 1$ for $\uparrow, \downarrow$

& $c_{k\sigma} = \sum_i c_{i\sigma} e^{ik \cdot r}$

For $Q = (\pi, \pi) = G/2$ = half of the reciprocal lattice vector. This breaks the lattice translational symmetry - doubling the unit cell in real space and reducing the reciprocal lattice by half in this case.



AFM



- So, in real space spins are staggered, with ↑ & ↓ spins in alternating sites. Therefore, the new unit cell, called AFM / magnetic unit cell now has two basis states, ↑ & ↓ spin atoms, so we have a 2-sublattice basis in the Hamiltonian and in the spinor state. Sometimes they are denoted by A & B sublattice, for convenience, and the magnetization per unit cell is now defined as

$$m = \langle S_z^A \rangle - \langle S_z^B \rangle \quad \text{---(21c)}$$

$$= \frac{1}{2} \langle [n_{i\uparrow}^A - n_{i\downarrow}^A) - (n_{i\uparrow}^B - n_{i\downarrow}^B)] \rangle \quad \text{---(21d)}$$

So, the total magnetization of the unit cell is zero in the ideal antiferromagnetic case, but spins are ordered in the ground state at each site.

(*) We can insert the mean-field ansatz in the Hubbard model in either real or momentum space, and yield the same result.

$$\mathcal{H}_V = -\frac{U}{2N}\sum_q \left[\langle S_s(Q)\rangle + S_s(Q)\right]\left[\langle S_s(-Q)\rangle + S_s(Q)\right]\delta_{Q,q}$$

$$\approx -U\langle S_s(Q)\rangle S_s(Q) - U\langle S_s(Q)\rangle^2, \qquad \because S_s(-Q) = S_s(Q)$$

$$= -U\sum_k m\left[c^\dagger_{k+Q\uparrow}c_{k\uparrow} - c^\dagger_{k+Q\downarrow}c_{k\downarrow}\right] - Um^2, \quad \text{at } Q=(\pi,\pi,\pi) \qquad \cdots (22)$$

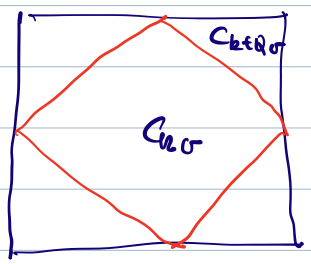
The full Hamiltonian is

$$H_{SDW} = \sum_{k,\sigma}\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma} + H_V.$$

$$= \sum_{k\in MBZ,\sigma}\left[\varepsilon_k c^\dagger_{k\sigma}c_{k\sigma} + \varepsilon_{k+Q}c^\dagger_{k+Q\sigma}c_{k+Q\sigma}\right]$$

$$- Um\sum_{k\in MBZ,\sigma}\sigma\, c^\dagger_{k+Q\sigma}c_{k\sigma} - Um^2 \qquad \cdots (23)$$

where we have restricted the k-values within the magnetic Brillouin zone, and the one outside is defined to be c_{k+Q}.



The Hamiltonian in eq (23) is not diagonal in this mean field theory, and is of the form $H = \sum_{\alpha\beta} \varepsilon_{\alpha\beta} c_\alpha^\dagger c_\beta$, that we studied in the second quantization chapter. To diagonalize it we invoke the same canonical transformation, by the unitary transformation which diagonalize the Hamiltonian matrix.

- We define the spinor $\psi_{k,\sigma} = (c_{k\sigma} \;\; c_{k+Q\sigma})^T$, and then we express the Hamiltonian in the matrix form

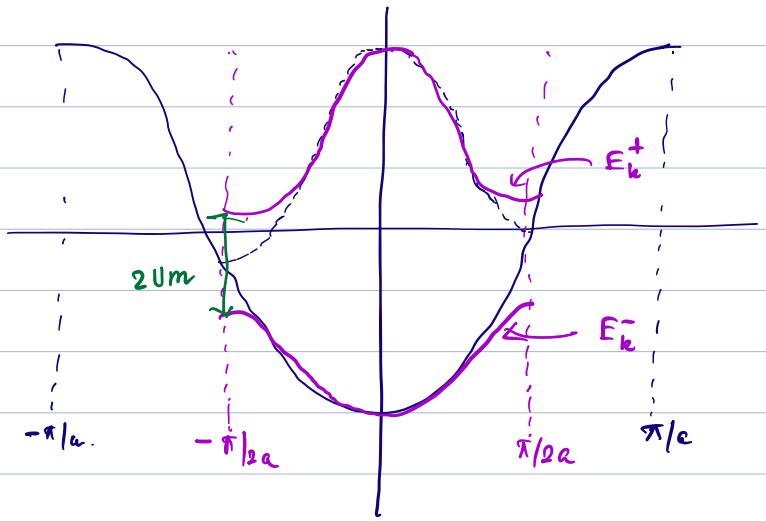
$$H_{SDW} = \sum_{k,\sigma} \psi_{k\sigma}^\dagger \, H_{SDW}^\sigma(k) \, \psi_{k\sigma}$$

where $$H_{SDW}^\sigma(k) = \begin{pmatrix} \varepsilon_k & -\sigma Um \\ -\sigma Um & \varepsilon_{k+Q} \end{pmatrix} \quad \text{--- (24)}$$

We can diagonalize this 2×2 matrix for each spin separately. The eigenvalues are

$$E_{k,\sigma}^\pm = \varepsilon_k^+ \pm \underbrace{\sqrt{(\varepsilon_k^-)^2 + (Um)^2}}_{E_{ok}}, \quad \varepsilon_k^\pm = \frac{\varepsilon_k \pm \varepsilon_{k+Q}}{2} \quad \text{-- (25)}$$

This is like the nearly free electron model, in which, the parabolic bands are folded within the reciprocal lattice defined by G, and at the zone boundary, a gap opens. In the present case, the band in a reciprocal lattice G is now folded inside a reduced magnetic Brillouin zone at $Q = G/2$, and a magnetic gap of $2\cdot Um$ opens at the mag. BZ boundary.



Now, we have two bands inside the magnetic BZ, while we started with only one band. If we set the momentum density $\langle n_k \rangle = 1$ at $T=0$ at all k upto the fermi level, we may get larger number of electrons in two bands. But the number of electrons must remain the same. What happen is that the occupation density at each k is now not identically 1, but have a probability distribution of $\langle n_k \rangle = |v_k|^2 \leq 1$ where v_k is the component of the eigenvector of $H_{SDW}^{\sigma}(k)$. We also have to reevaluate the chemical potential to maintain the same number of electrons.

The two eigenvectors are denoted by

$$\psi_+^{\sigma}(k) = \begin{pmatrix} \alpha_k \\ \sigma \beta_k \end{pmatrix}, \quad \psi_-^{\sigma}(k) = \begin{pmatrix} -\sigma \beta_k \\ \alpha_k \end{pmatrix} \qquad \cdots (26a)$$

The normalization condition gives $|\alpha_k|^2 + |\beta_k|^2 = 1$. Because of this constraint, α_k & β_k can be parameterized by a single angular variable θ_k as $\alpha_k = \cos\theta_k$, $\beta_k = \sin\theta_k$. We will however continue with α_k & β_k.

Solving the Hamiltonian we get

$$|\alpha_k| = \sqrt{\frac{1}{2}\left(1+\frac{\varepsilon_{ik}^-}{E_{0k}}\right)} \; ; \; |\beta_k| = \sqrt{\frac{1}{2}\left(1-\frac{\varepsilon_{ik}^-}{E_{0k}}\right)} \quad --(26b).$$

The canonical transformation from c, c^+ to b, b^+ which destroy and create a quasiparticle in the bands are now expressed as

$$b_{k\sigma+} = \alpha_k c_{k\sigma} - \sigma \beta_k c_{k+Q,\sigma} \quad --(27a)$$

$$b_{k\sigma-} = \sigma \beta_k c_{k\sigma} + \alpha_k c_{k+Q\sigma} \quad --(27b).$$

The inverse transformation is

$$c_{k\sigma} = \alpha_k b_{k\sigma+} + \sigma \beta_k b_{k\sigma-} \quad --(27c)$$

$$c_{k+Q,\sigma} = -\sigma \beta_k b_{k\sigma+} + \alpha_k b_{k\sigma-} \quad --(27d)$$

The Hamiltonian is diagonal in this basis as

$$H_{SDW} = \sum_{k,\sigma,\nu=\pm} E_{k\sigma}^{\nu} b_{k\sigma\nu}^{+} b_{k\sigma\nu} \quad --(28).$$

The ground state (mean field) wavefunction is

$$|\psi_{SDW}\rangle = \prod_{k \in k_{F,\sigma}} b_{k\sigma+}^{+} b_{k\sigma-}^{+} |0\rangle \quad --(29).$$

- With this ground state, we have to re evaluate the chemical potential to maintain the number of particles to be fix, and the staggered magnetization m from eq(21a).

- The number of electron (per unit cell).

$$n = (n_\uparrow + n_\downarrow)$$

$$= \sum_{k \in MBZ, \sigma} \langle \psi_{SDW} | \left(c^\dagger_{k\sigma} c_{k\sigma} + c^\dagger_{k+Q\sigma} c_{k+Q\sigma} \right) | \psi_{SDW} \rangle$$

[in thermal equilibrium.]

Now using the canonical transformation of eqn (27c) & (27a), we get

$$c^\dagger_{k\sigma} c_{k\sigma} + c^\dagger_{k+Q\sigma} c_{k+Q\sigma} = |\alpha_k|^2 b^\dagger_{k\sigma+} b_{k\sigma+} + |\beta_k|^2 b^\dagger_{k\sigma-} b_{k\sigma-}.$$

Hence $$n = \sum_{k \in MBZ, \sigma} \left[|\alpha_k|^2 \underbrace{\langle b^\dagger_{k\sigma+} b_{k\sigma+} \rangle}_{f(E_k^+)} + |\beta_k|^2 \underbrace{\langle b^\dagger_{k\sigma-} b_{k\sigma-} \rangle}_{f(E_k^-)} \right]$$

$$= 2 \sum_{k \in MBZ} \left[|\alpha_k|^2 f(E_k^+) + |\beta_k|^2 f(E_k^-) \right] \quad \text{--(30a)}$$

for spin.

$$= 2 \sum_{k < k_F} \left(|\alpha_k|^2 + |\beta_k|^2 \right) \quad \text{As } T \to 0,\ f(\varepsilon) \to 1. \quad \text{--(30b)}$$

For all the k-points in both E_k^+ & E_k^- are filled, we get $|\alpha_k|^2 + |\beta_k|^2 = 1$, otherwise only the weight of the corresponding filled band contributes.

- The other self-consistent equation is the magnetization one, from eqn 21(a)

$$m = \frac{1}{2} \sum_{k,\sigma} \langle c^\dagger_{k+Q\sigma} c_{k\sigma} \rangle = \sum_{k \in MBZ} \langle \psi_{SDW} | c^\dagger_{k+Q} c_k | \psi_{SDW} \rangle$$

for any one spin.

$$\langle \psi_{SDW} | c^\dagger_{k+Q} c_k | \psi_{SDW} \rangle = \langle \psi_{SDW} | \left(-\beta^*_k b^\dagger_{k+} + \alpha^*_k b^\dagger_{k-} \right) \left(\alpha_k b_{k+} + \beta_k b_{k-} \right) | \psi_{SDW} \rangle$$

$$= -\alpha_k \beta^*_k \underbrace{\langle b^\dagger_{k+} b_{k+} \rangle}_{f(E_k^+)} + \alpha^*_k \beta_k \underbrace{\langle b^\dagger_{k-} b_{k-} \rangle}_{f(E_k^-)}$$

$$- |\beta_k|^2 \underbrace{\langle b^\dagger_{k+} b_{k-} \rangle}_{=0} + |\alpha_k| \underbrace{\langle b^\dagger_{k-} b_{k+} \rangle}_{=0 \text{ in the SDW state}}$$

$$\therefore \quad m = \sum_{k \in MBZ} \left[-\alpha_k \beta_k^* f(E_k^+) + \alpha_k^* \beta_k f(E_k^-) \right].$$

For those $k \in k_F$ values, where both bands are filled (at $T \to 0$), and since α_k & β_k are real, so, the contribution to 'm' vanishes. Only those k-points where only the filled band contributes.

$$= \sum_{k \in MBZ} \left[-\frac{Um}{E_{0k}} f(E_k^+) + \frac{Um}{E_{0k}} f(E_k^-) \right]$$

$$= Um \sum_{k \in MBZ} \frac{1}{E_{0k}} \left(f(E_k^-) - f(E_k^+) \right)$$

or, $$1 = 2U \sum_{k \in MBZ} \frac{\left(f(E_k^-) - f(E_k^+) \right)}{E_k^+ - E_k^-} \quad \text{---(31a)}$$

where $E_k^+ - E_k^- = 2E_{0k}$ and $\varepsilon_{k+Q} = -\varepsilon_k$ at $Q = (\pi, \pi, \pi)$

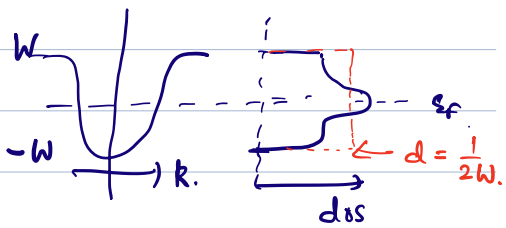
$$\Rightarrow \quad \boxed{1 = -U \chi_s(Q, 0)} \quad \text{---(31b)}$$

(The factor of 2 arises in going from MBZ to the full BZ.)

We again see that the self consistent gap equation is same as the Stoner criterion but at $q = Q$.

Both eq (30a) and (31b) is to be computed self-consistently as a function of μ and U. If a solution exists, then an SDW state can form. With lot of low-energy approximation, one may obtain some analytical expression for the two self-consistent solutions, which may eventually not be very useful. One can solve these equations numerically.

To semi-quantitatively proceed, we assume the density of state is uniform in energy, ranging from $-W$ to W, where W is the bandwidth ($= 6t$ for the tight binding case). Then eqn (31) gives



$W = 6t$.

$$\frac{1}{U} = -\int_{-\infty}^{\infty} d\varepsilon \; d(\varepsilon) \; \frac{1}{\sqrt{\varepsilon^2 + (Um)^2}} \left[f\left(\varepsilon_f - \sqrt{\varepsilon^2 + (Um)^2}\right) - f\left(\varepsilon_f + \sqrt{\varepsilon^2 + (Um)^2}\right) \right]$$

where we focus in the vicinity of the gap where $\varepsilon_{k+Q} = -\varepsilon_k$ such that $\varepsilon_k^+ = \varepsilon_f$ and $\varepsilon_k^- = 2\varepsilon_k$ and $E_{ok} = \sqrt{\varepsilon^2 + (Um)^2}$.

$$= -\frac{U}{2W} \int_{-W}^{\varepsilon_f} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + (Um)^2}} \; \theta\left[\varepsilon_f - \sqrt{\varepsilon^2 + (Um)^2}\right]$$

at $T \to 0$, $f\left(\varepsilon_f + \sqrt{\varepsilon^2 + (Um)^2}\right) \to 0$

& $f\left(\varepsilon_f - \sqrt{\varepsilon^2 + (Um)^2}\right) \to 1$.

$$\approx -\frac{1}{2W} \int_{-W}^{\varepsilon_f} \frac{d\varepsilon}{\varepsilon}$$

$$= -\frac{1}{2W} \ln\left(\varepsilon_f / W\right)$$

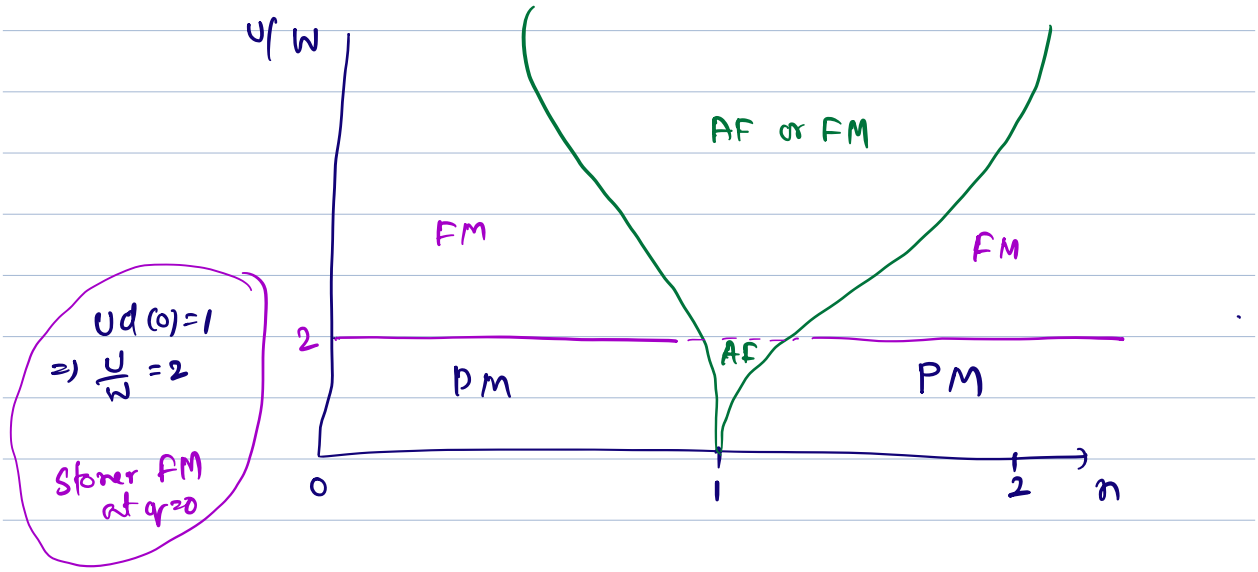
$\varepsilon_F = W/2$ is the half-filling case, i.e., $n = 1$.

or, $$\boxed{U = -\frac{2W}{\ln(n-1)}} \quad -- (32)$$

when $Q = 2k_F$

The singularity in the Fermi surface is now converted into a singularity with respect to the carrier density. The critical value of U to have a phase transition is when the RHS gives zero. This happens at three filling fraction of $n = 1$ when $\log(0) \to -\infty$ and $U \to 0$. Therefore an AFM instability is expected near the Half filling.

The qualitative phase diagram can then be drawn as


U/W
AF or FM
FM
FM
2
AF
PM
PM
0
1
2
n
Ud(0)=1
⇒ U/W = 2
Stoner FM
at q=0

5.5 $U \to \infty$ limit : Mott insulator

[P. Phillips book
P. Coleman book]

In the above we discussed the Fermi surface instability at two characteristic wavevectors and the corresponding phase transitions to the FM and the AFM phases. Then we developed the mean field theory in the momentum space by going from $n_{k\sigma} \to \langle n_{k\sigma} \rangle + \delta n_{k\sigma}$. This approximation is valid in the weak coupling limit where $U/2W \leq 1$.

In the strong coupling limit of $U/W \to \infty$, the localized picture arises - which is in general classified as Mott insulator. In some commensurate filling factor, we however see the ordering in charge or spin density. Because of the real space picture, we get energy levels, or flat band in the momentum space. As the hopping is introduced the electrons can now hop between the sites and hence $n_{i\sigma}$ is no longer a conserved quantity. Here we can think about a mean field theory by expanding $n_{i\sigma} \to \langle n_{i\sigma} \rangle + \delta n_{i\sigma}$. We will first discuss such a mean field theory, which will result in producing dispersion in the energy levels.

Typically, $U/W \to \infty$ limit is rarely reached in real materials - although in several materials such as V_2O_3, cuprate superconductors and in Heavy fermion compounds, such strong coupling limit and AFM insulating phase is believed to exist. But nowadays such strong coupling limit is easily achieved and tuned in cold atom systems and hence the Mott insulating, Wigner crystal and other phases are or can be observed.

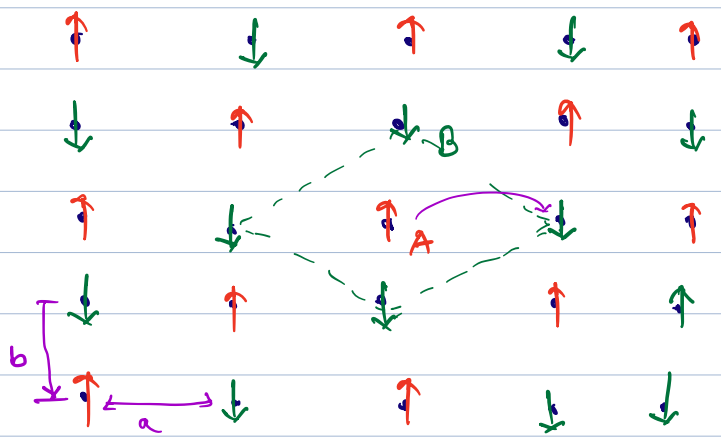
After developing the mean-field theory, we will focus on a powerful method to construct the so-called effective or renormalized method for the low-energy physics. The method is general to the degenerate perturbation theory to quasi degenerate perturbation theory. This method is used widely in strong coupling theory and also in other contexts and sometimes known as the Schrieffer-Wolf method. Using this method the Hubbard model can be shown to give a low energy t-J model.

5.5A Mean field Theory of AFM in $U \to \infty$ limit.

As we argued in the introduction, there is a preferred AFM state at half-filling, ie, $n=1$, where every lattice site has one electrons. Due to coulomb repulsion, they prefer to be one electron per site. At $t=0$, this makes the ground state energy level to be $-\mu N$, with $2N$-fold degeneracy, and the first excited state is $-\mu N + U$, with one site being doubly filled, and so on. This is the Mott insulating state.

This Mott insulating state with 2-fold spin degeneracy is very unstable to any finite value of the nearest neighbor hopping $t > 0$. Slater, using the Hartree-Fock theory, showed that the Mott phase becomes AFM state at $t \to 0^+$. To establish that we will use a mean field theory, but starting from the real space.

The AFM order looks like



we denote the up and down spin states on A & B sites. The unit cell now contains two sublattice basis. We define a doubled unit cell which contain two sublattices with

opposite spin, and denote the unit cell by the index I. Therefore at the same unit cell I, the magnetization is defined by

$$m_I = m_A - m_B$$

This is called the staggered magnetization.
This should be contrasted with the local (onsite) magnetization as $m_A = \frac{1}{2}(\rho_{iA\uparrow} - \rho_{iA\downarrow})$ & $m_B = \frac{1}{2}(\rho_{iB\uparrow} - \rho_{iB\downarrow})$. We are however going to focus on the staggered magnetization as the order parameter here. In the AFM phase we have $m_A = -m_B$ in each I. Then the staggered magnetization is related to the local magnetic moment as

$$m_I = m_A - m_B = 2\, m_A.$$

where the total magnetic moment $m_I^{tot} = m_A + m_B = 0$.

We will assume uniform magnetization in all unit cell, i.e., $m_I = m = \frac{m_A}{2} = -\frac{m_B}{2}$ in all unit cell.

Now we expand the densities around the mean value of the magnetization as

$$\left.\begin{aligned} \rho_{IA\uparrow} &= m + \delta\rho_{IA\uparrow} \\ \rho_{IA\downarrow} &= -m + \delta\rho_{IA\downarrow} \end{aligned}\right\} \quad \cdots (33a)$$

and

$$\left.\begin{aligned} \rho_{IB\uparrow} &= -m + \delta\rho_{IB\uparrow} \\ \rho_{IB\downarrow} &= m + \delta\rho_{IB\downarrow} \end{aligned}\right\} \quad \cdots (33b)$$

↑ number ↑ operators.

Then using the mean-field decomposition of the Hubbard model, we get

$$H_U = \frac{U}{V}\sum_I \left[(m+\delta\rho_{IA\uparrow})(-m+\delta\rho_{IA\downarrow}) + (-m+\delta\rho_{IB\uparrow})(m+\delta\rho_{IB\downarrow})\right]$$

$$= -\frac{U}{V} m \sum_I (\delta\rho_{IA\uparrow} - \delta\rho_{IB\uparrow}) + (\uparrow \to \downarrow) - 2Um^2$$

$$= -\frac{Um}{V}\sum_I \left(c^\dagger_{IA\uparrow} c_{IA\uparrow} - c^\dagger_{IB\uparrow} c_{IB\uparrow}\right) + (\uparrow\to\downarrow) - 2Um^2.$$

$$= Um \sum_{k,\sigma} \left(c^\dagger_{kB\sigma} c_{kB\sigma} - c^\dagger_{kA\sigma} c_{kA\sigma}\right) - 2Um^2.$$

where $\sum \rho_{IA\sigma} = \sum_{kk'} c^\dagger_{kA\sigma} c_{k'A\sigma} \sum_I e^{i(k-k')\cdot R_I} = \sum_k c^\dagger_{kA\sigma} c_{kA\sigma}$

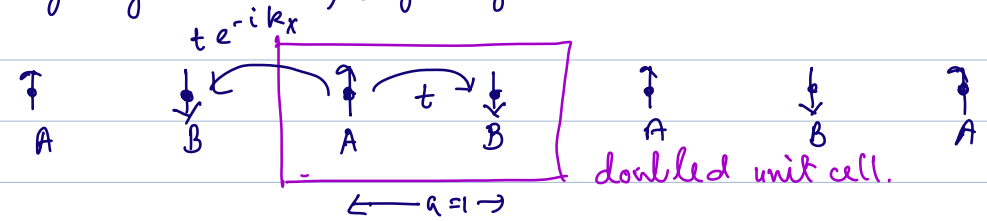
- The kinetic energy term is

$$H_K = -t \sum_{\langle ij\rangle,\sigma} c^\dagger_{i\sigma} c_{i\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}$$

$$= -t \sum_I \left(c^\dagger_{IA\sigma} c_{IB\sigma} + h.c.\right) - \mu \sum_{I,\sigma} (n_{IA,\sigma} + n_{IB,\sigma})$$

$$= \sum_{k\sigma} \varepsilon_k \left(c^\dagger_{kA\sigma} c_{kB\sigma} + h.c\right) - \mu \sum_{k,\sigma} \left(c^\dagger_{kA\sigma} c_{kA\sigma} + c^\dagger_{kB\sigma} c_{kB\sigma}\right)$$

Note that the dispersion relation ε_k is modified here compared to the original unit cell because of the zone folding. Along any direction, say along the x-direction we have



So, $\varepsilon_k = t(1+e^{-ik_x}) + t(1+e^{-ik_y}) + t(1+e^{-ik_z})$

$$= 3t + 6t(\cos k_x + \cos k_y + \cos k_z) - i\,6t(\sin k_x + \sin k_y + \sin k_z)$$

- To formulate the Hamiltonian in a matrix form, we define the spinor $\Psi_{k\sigma} = (c_{kA\sigma} \;\; c_{kB\sigma})^T$, which gives

$$H = H_K + H_U = \sum_{k\sigma} \Psi^\dagger_{k\sigma} H_{k\sigma} \Psi_{k\sigma} - U m^2 N$$

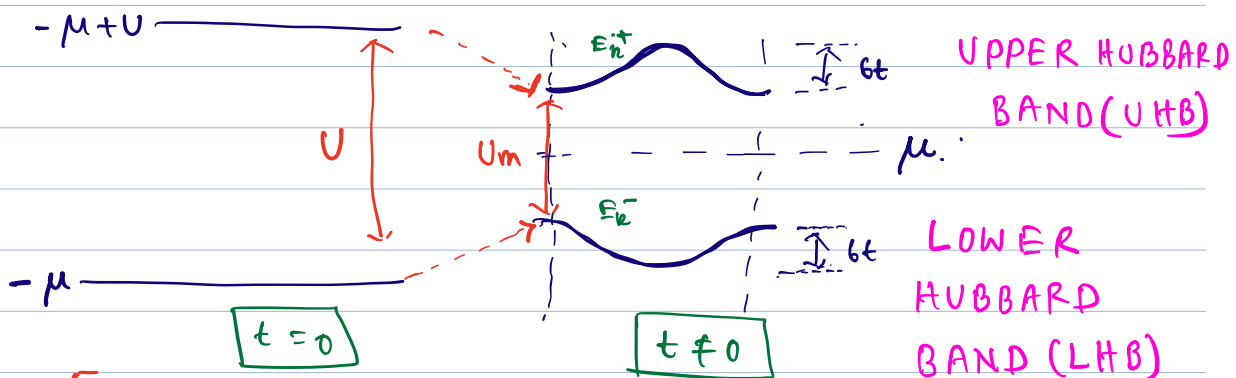
where $$H_{k\sigma} = \begin{pmatrix} -\mu - Um & \varepsilon_k \\ \varepsilon_k & -\mu + Um \end{pmatrix} \quad \text{--- (34)}$$

Notice that this Hamiltonian is very different from both FM & AFM mean field Hamiltonians defined in the momentum space. Here the magnetic gap enters into the diagonal term like a "Zeeman term", while the kinetic energy ε_k (without the chemical potential) goes into the off diagonal term.

The eigenenergies are

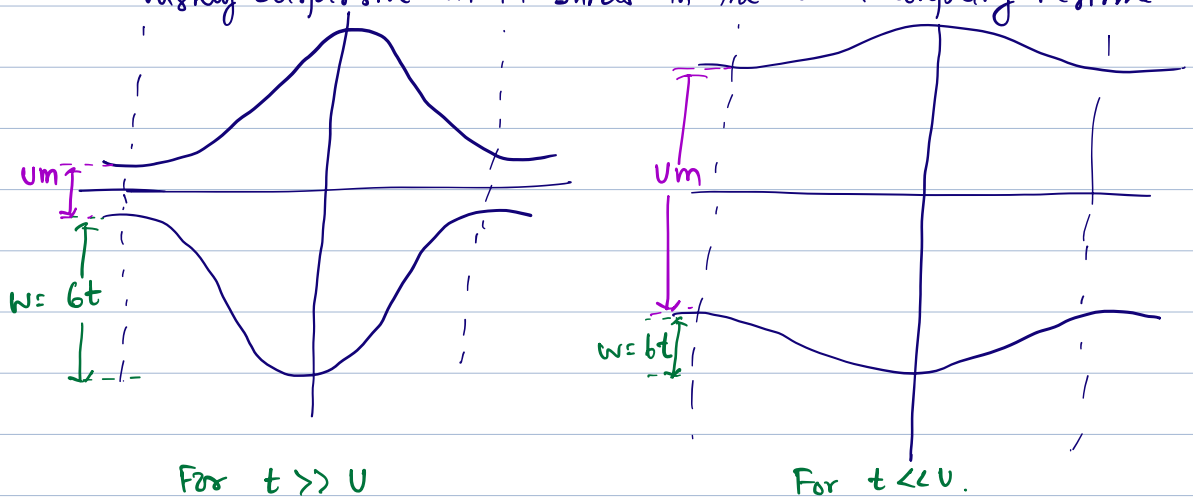
$$E^\pm_k = -\mu \pm \sqrt{\underbrace{|\varepsilon_k|^2}_{E_{0k}} + (Um)^2} \quad \text{--- (35)}.$$

This splits the single particle energy $-\mu$ in the MoH limit into two bands $E^\pm_k$, with an anisotropic gap of $\Delta_k = \sqrt{\varepsilon_k^2 + (Um)^2}$.



H.W. Find the range of μ where a metallic phase can appear.

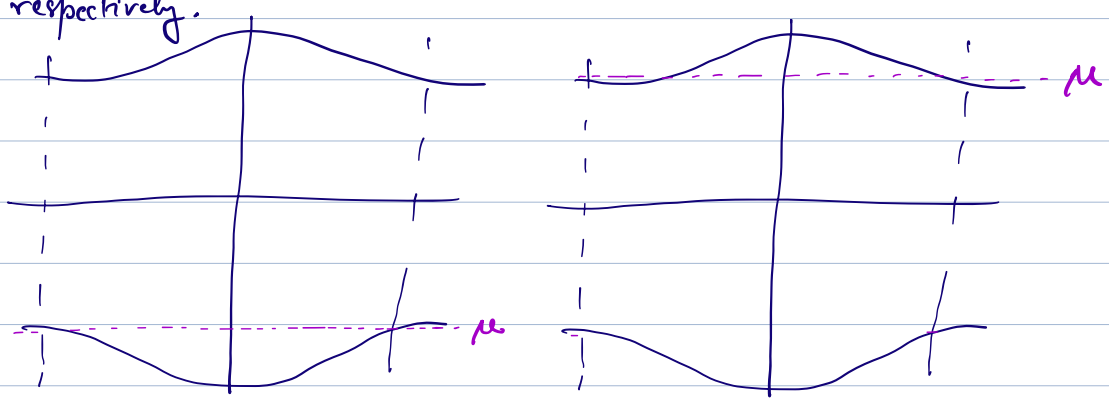
- This weakly dispersive Hubbard bands can be contrasted with the highly dispersive AFM bands in the weak coupling regime:



For $t \gg U$ For $t \ll U$.

- Correlated Metals (semi metals).

If we add a few holes or electrons to the Mott insulator state ($t \ll U$), the chemical potential crosses the LHB or UHB respectively.



hole doping. electron doping.

Here the Fermi surface is very tiny and the carrier concentration (ie. the number of particles on the Fermi surface) is very small, and we will get semi-metallic like phase. (Note that for dilute hole doping, we get Nagaoka ferromagnetism, not a Stoner ferromagnetism.

- The eigenvectors are obtained (in similar notation as in the AFM case) as:

$$\psi^{+}_{k\sigma} = \begin{pmatrix} \alpha_k \\ \sigma \beta_k \end{pmatrix}, \quad \psi^{-}_{k\sigma} = \begin{pmatrix} -\sigma \beta_k \\ \alpha_k \end{pmatrix}$$

where $|\alpha_k| = \sqrt{\frac{1}{2}\left(1 - \frac{Um}{E_{0k}}\right)}$, $|\beta_k| = \sqrt{\frac{1}{2}\left(1 + \frac{Um}{E_{0k}}\right)}$

- The self consistent magnetic gap equation is

$$m = \frac{1}{2N} \sum_{I,} \langle (n_{IA\uparrow} - n_{IB\downarrow}) \rangle$$

$$= \frac{1}{2} \sum_{k \in BZ} [\langle n_{kA\uparrow} \rangle - \langle n_{kB\downarrow} \rangle] \qquad [\text{factor 2 for spin}$$

$$= \frac{1}{2} \sum_{k} \left[|\beta_k|^2 f(E^{-}_k) - |\alpha_k|^2 f(E^{+}_k) \right] \qquad [\text{we extend the summation to entire BZ with a factor of 2}]$$

We assume that at half-filling we have an AFM insulator so that the only filled band is the E^{-}_k. Then we get

$$= \frac{1}{2} \sum_{k} \frac{1}{2} \left(1 + \frac{\Delta}{\sqrt{\varepsilon_k^2 + \Delta^2}}\right) \qquad \Delta = Um$$

$$= \frac{1}{4} + \frac{1}{4} \sum_{k} \frac{1}{\sqrt{1 + \frac{\varepsilon_{ak}^2}{\Delta^2}}}$$

$$= \frac{1}{4} + \frac{1}{4} \sum_{k} \left(1 - \frac{|\varepsilon_{ak}|^2}{2\Delta^2}\right) + O\left(\frac{1}{\Delta^4}\right)$$

[Notice that we set $\sum_k 1 = 1$ because there is an implicit normalization of $\frac{1}{V_{BZ}} \sum_k 1 = 1$.]

$$= \frac{1}{2} - \frac{4t^2}{8\Delta^2} \underbrace{\sum_k |g(k)|^2}_{\#}, \quad \text{where } g(k) = \varepsilon(k)/t.$$

$\because \varepsilon_k = -2t(\cos k_x + \cdots)$

$$\approx \frac{1}{2}\left(1 - \frac{1}{2}\frac{t^2}{\Delta^2} \#\right)$$

Such equations can be solved iteratively by substituting m on the R.H.S and doing a leading order expansion but only keep the terms upto the same order:

$$m = \frac{1}{2}\left(1 - \frac{\#}{2}\frac{t^2}{U^2}\frac{4}{\left(1-\frac{\#}{2}\frac{t^2}{\Delta^2}\right)^2}\right)$$

$$= \frac{1}{2}\left[1 - 2\#\frac{t^2}{U^2}\left(1+\frac{\#}{2}\frac{t^2}{\Delta^2}\right)^{-2} + \cdots\right]$$

$$= \frac{1}{2}\left[1 - 2\#\frac{t^2}{U^2} + \Theta\left(\frac{t^4}{\Delta^4}\right)\right]$$

- we can calculate the total energy similarly:

$$E = \sum_k \left[\underbrace{E_k^+ f(E_k^+)}_{=0} + \underbrace{E_k^- f(E_k^-)}_{=1}\right] - Um^2 \quad \text{at } T=0.$$

$$= \sum_k \left[-\mu - \Delta\sum_k \sqrt{1+\frac{\xi_k^2}{\Delta^2}} - Um^2\right]$$

$$= E_0 - \Delta\sum_k \left(1 + \frac{\xi_k^2}{2\Delta^2} + \cdots\right) - Um^2$$

$$= E_0 - \Delta - \frac{\Delta}{2\Delta^2}\#\frac{4t^2}{} - Um^2$$

$$= E_0 - Um - 2\#\frac{t^2}{Um} - Um^2$$

$$= E_0 - U\frac{1}{2}\left(1-2\#\frac{t^2}{U^2}\right) - 4\#\frac{t^2}{U}\left(1+2\#\frac{t^2}{U^2}+\cdots\right) - \frac{U}{4}\left(1-2\#\frac{t^2}{U^2}\right)^2$$

$$= E_0 - \frac{U}{2} - \frac{3\#}{8}\underbrace{\frac{4t^2}{U}}_{J} + \Theta(t^4/U^3)$$

Therefore, we see that the correction comes in the 2nd order correction term as $J = 4t^2/U$. For $J>0$, we will have an instability in the energy in the 2nd order perturbation term, ie some singularity arises in the energy as we go to 2nd order perturbed energy. Below we construct t-J model.

5.6 Effective / Renormalized Hamiltonian method

By effective or renormalized Hamiltonian, we generally mean a low-energy Hamiltonian for the states at low-energy (ground state) which is our interest. If we have only one state (ground state) or a degenerate ground state, we generally consider a perturbation theory to obtain correction to this energy state. Then the perturbation theory converges if this state is well separated in energy from the first excited state. But if we have a "bunch" of states - namely a manifold of quasi-degenerate states at low energy which are separated from the other states with large energy gap, then we cannot really find energy corrections to each energy levels this way, since there will be off-diagonal terms. Rather we want to obtain a Hamiltonian matrix - called effective Hamiltonian - only defined for the low-energy manifold of states. So, this seems like a perturbation theory, but slightly more general than the perturbation theory. (In fact, in the renormalization group (RG) theory, we do a similar technique - that we start with a interacting theory, and then want to obtain a low-energy theory. A low-energy theory for bosons is a long wavelength (or $k \to 0$) modes or for bosons long-wavelength fluctuations around the Fermi momenta ($k \to k_F + \delta k$) theory. Here we want to get rid of the high-energy (large k) modes and obtain an effective/renormalized theory for the low-energy mode. Here also the above method would be applicable with perhaps slight adjustment in the theory).

This effective Hamiltonian method is more powerful and general than only to finding low-energy effective theory of a given Hamiltonian. Imagine, we have two distinct degrees of freedom such as electrons and nucleus or electrons and phonon. Then the total Hamiltonian has electronic part, other degrees of freedom (nucleus / phonon) and a coupling term. Then we want to obtain an effective Hamiltonian for the electronic part only by "integrating out" the other degrees of freedom. This is in the spirit of treating the coupling part perturbatively (or sometimes exactly) such that both the electronic and phonon part become very much decoupled at the cost of having corrections to the electronic Hamiltonian and the phonon Hamiltonian. Then we can simply work with the electronic Hamiltonian of our interest. Similar situation arises in open quantum systems where we have a system of our interest, and a bath or environment and a coupling between them. Here also we can apply a similar method and obtain an effective Hamiltonian for our system of interest.

We are learning it in the context of the Hubbard model, because in the strong coupling limit of $U/t \to \infty$, at half-filling $n=1$, we see that there is no unoccupied site or state as doubly occupied site / state cost $U \to \infty$ energy. Therefore, the singly occupied states of up and down spins are well separaseparated in energy from the doubly occupied and empty state. The effective Hamiltonian for the two low-energy spin-up and spin down states turns out to be a Heisenberg-like Hamiltonian called the 't-J'.

model. We want to derive such a model. A similar derivative is also applicable in the Heavy fermions compound where one has a strongly correlated / localized f-orbital state and a delocalized / itinerant conduction bands. Such a model is called Periodic Anderson Lattice model. A similar effective Hamiltonian for the low-energy singly occupied f-orbital model gives the well-known the Kondo Lattice model. This mapping between the two models is known as the Schrieffer-Wolf model.

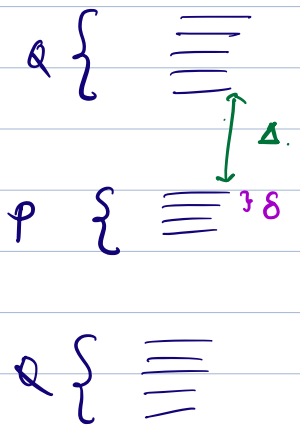
We will start with developing the theory as general as possible, and then apply for the Hubbard model here and for the electron-phonon coupling model in the next chapter.

We have a total Hamiltonian that we decompose as

$$H = H_0 + V \qquad --(1)$$

where H_0 is the independent "system" + "bath" part of the Hamiltonian and V is the interaction between them.

Then the eigenstates of the "independent part H_0 has well separated manifolds as shown here, in which the 'P' states are the states of our interest, which we denote as "low-energy states" although it does not necessarily have to be low-energy states, but states of our interest. We denote the remaining states by "Q". The states in P can be degenerate -



then we can simply use degenerate perturbation theory, or have energy gap $\delta << \Delta$, where Δ is the gap from this P manifold to the rest of the states on both sides (or P states can simply be the lowest energy states and they are separated from the high energy states by a gap Δ).

procedure

There is an exact theoretical to do this, but becomes analytically it becomes difficult and we eventually make perturbation theory like approximation. The exact procedure goes as follows. Let us say P is a projection operator on the manifold states of our interest (ex, P-states) and defined as

$$P = \sum_{p \in P} |p\rangle\langle p| \quad \text{--- (2a)}$$

Then the remaining states form an orthogonal projection operator,

$$Q = \sum_{q \in Q} |q\rangle\langle q|. \quad \text{--- (2b)}$$

$|\psi_i\rangle$ states are the eigenstates of H_0.

Because $|\psi_i\rangle$ states form a complete basis, so, $P+Q=\mathbb{I}$, and $P^2 = P$, $Q^2 = Q$ and $PQ = QP = 0$, which are the consequence of the orthonormalization of the states $|i\rangle$.

Now, there is a general theorem, possibly proved by Van Vleck, that the "interaction" operator can be written as

$$V = V_D + V_X, \quad \text{---- (3a)}$$

where V_D is "diagonal" or decoupled or projected in the P & Q-states

$$V_D = PVP + QVQ, \quad \text{-- (3b)}$$

and V_X is the off diagonal part:

$$V_X = PVQ + QVP \quad \text{-- (3c)}$$

Then, we want to find a unitary operator $U = e^{iS}$. where S is an Hermitian operator, such that in the rotated basis of $P' = U^{+}P$, $Q' = U^{+}Q$, the off diagonal part $V_X = 0$. The remaing problem now is to find such an Hermitian operator S.

This problem in turn says find an operator S, which reduces the total Hamiltonian H to an effective Hamiltonian H_{eff} in which P & Q manifold are decoupled as.

$$e^{iS}\underbrace{(H_0 + V)}_{H} e^{-iS} = H_{eff} \quad \text{--- (4a)}$$

where

$$P H_{eff} Q = Q H_{eff} P$$
$$= \sum_{p,q} |p\rangle\langle q| (H_{eff})_{pq} = 0$$

$$\Rightarrow \langle p| H_{eff} |q\rangle = 0. \quad \text{--- (4b)}$$

- Using the Becker-Cambell-Hausdroff formula we obtain an series of commutator as

$$H_{eff} = H_0 + V + i[S, H] + \frac{i^2}{2!}[S,[S,H]] + \frac{i^3}{3!}[S,[S,[S,H]]] + \cdots$$
$$\approx H_0 + \underbrace{V + i[S, H_0]}_{=0} + i[S,V] - \frac{1}{2}[S,[S,H_0]] + \underbrace{\theta(V^3)}_{\cdots}. \quad \text{(5a)}$$

where we truncate the series at the 2nd-order term in the interaction term V, as this is like a 2nd order perturbation theory.

Next we want to choose 'S' such that

$$\boxed{V + i[S, H_0] = 0.} \quad \text{--- (5b)}.$$

substituting eq(5b) in eq(5a), we get

$$\boxed{H_{eff} \approx H_0 + \frac{i}{2}[S, V]} \quad \text{--- (5c)}.$$

(In some literature, such as in Cohen-Tannoudji book, such an 2nd order term was obtained by expanding $S = S_0 + \lambda S_1 + \lambda^2 S_2 + \cdots$ and adding a λ in front of V as $H = H_0 + \lambda V$, and matching powers of λ on both sides.)

Now we obtain S from eqn (5b), by taking expectation value with respect to the eigenstates of H_0:

$$\langle p|V|q\rangle = -i\left[\langle p|SH_0|q\rangle - \langle p|H_0 S|q\rangle\right]$$
$$= -i\langle p|S|q\rangle(E_q^0 - E_p^0), \quad \forall\, p\in P,\ q\in Q,\ p\neq q$$

or

$$\langle p|iS|q\rangle = \frac{\langle p|V|q\rangle}{E_p^0 - E_q^0}, \quad p\neq q \qquad \cdots (5d)$$

$$= 0, \quad p = q. \ (\text{we choose } S \text{ to satisfy this})$$

Therefore, S is chosen to be completely off diagonal between the P & Q-manifolds, ie, S acts like a ladder or jump operator between the system (P) & bath (Q).

Now, we compute the matrix elements of H_{eff} in the P-states

$$\langle p|H_{eff}|p'\rangle = \langle p|H_0|p'\rangle + \frac{i}{2}\left[\langle p|S\underbrace{V}_{P+Q=\mathbb{I}}|p'\rangle - \langle p|V\underbrace{S}_{P+Q=\mathbb{I}}|p'\rangle\right]$$

Now, we insert $P+Q = \mathbb{I} = \sum_{k\in P+Q}|k\rangle\langle k|$, in the whose Hilbert space, and since $\langle p|S|k\rangle = 0$ for $k = p$, we only obtain obtain terms for $k\neq p$ as.

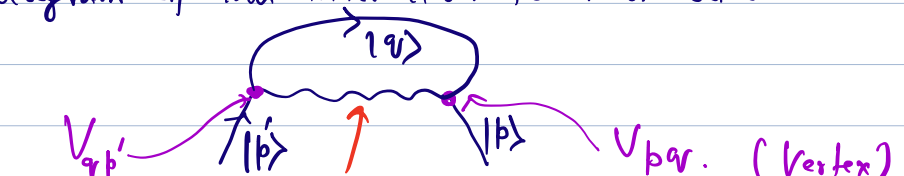
$$\boxed{(H_{eff})_{pp'} = E_p^0\delta_{pp'} + \frac{1}{2}\sum_q V_{pq}V_{qp'}\left[\frac{1}{E_p^0 - E_q^0} - \frac{1}{E_q^0 - E_{p'}^0}\right]} \qquad \cdots (5e)$$

where $V_{pq} = \langle p|V|q\rangle$.

This eq (5e) is very similar to the 2nd order perturbation theory, but now generalized for a manifold of states which need not be degenerate. For a degenerate case, $E^0_p = E^0_{p'}$, the two terms in the 2nd term will add up to the same term as we obtained in the QM course. For a single state $p = p'$, the matrix element of $V_{pq} = V^*_{qp}$ and we obtain exactly the same term as in the 2nd order perturbation theory.

The eigenvectors of H_{eff} will be different from those of H_0, and hence in this procedure we obtain corrections to both the energy eigenvalues E^0_p as well as to the eigenstates.

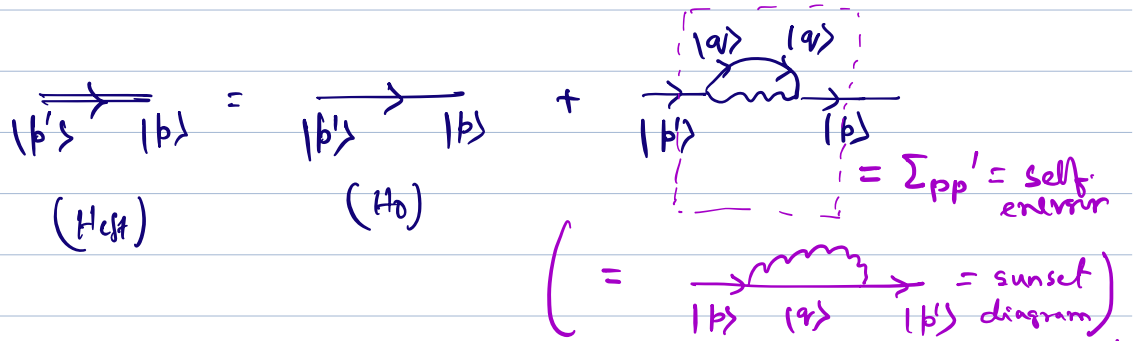
Notice that the perturbation term consists of $V_{pq} < V_{qp'}$ i.e., it consists of interaction between the low-energy (system) states and the high-energy (bath) states; one term $V_{p'q}$ scatter a state from $|p'\rangle$ to $|q\rangle$, followed by another scattering from $|q\rangle$ to $|p\rangle$. Therefore, this is like two-body interaction term between the states of H_0. A Feynmann diagram of this interaction term is like



"Propagator"

$$= \left[\frac{1}{E^0_p - E^0_q} - \frac{1}{E^0_q - E^0_{p'}}\right]$$

Then eq (5d) can be expressed in Feynmann diagram as



⚠ It might be obvious from eq (5e), but often people forget in other cases that the H_{eff} and H_0 are only defined in the restricted Hilbert space of P, not on the entire Hilbert space of P⊕Q. Sometimes, one use the full Hilbert space of P+Q, but insert the projection operator P in the expectation value calculation so that the only finite expectation value is for the $|\beta\rangle \in P$ states, and the rest is zero. This sort of treatment is sometimes called the Gutzwiller Projection method.

- t-J model: We will use this perturbation method for the Hubbard model to obtain the t-J model for the $|\uparrow\rangle$ & $|\downarrow\rangle$ states.
- Kondo model: H.W. Solve the Periodic Anderson model to obtain the Kondo model using this method.
- Electron-Phonon Coupling: In next chapter we will use this method to integrate out phonon modes and obtain an attractive electron-electron interaction giving superconductivity.

(similar method can be used to obtain the strong force between

proton-proton by integrating out the pion modes in a nucleus).

5.5.A The t-J model :

[G. Baskaran, P.W. Anderson].

We will now apply this Theory on the Hubbard model at half-filling in the $U/t \to \infty$ limit. Here of-course $H_0 = H_U$ is the unperturbed Hamiltonian and $V = H_t$ is the small perturbation. The low-energy manifold is singly occupied at all sites with energy $E_0 = -\mu N$. Then the first excited state is take one doubly occupied state and one empty state with energy $E_1 = -\mu N + UN$. The next state is 2-doubly occupied state and so on. Since $U \to \infty$, so, these manifolds are well separated.

Q $\equiv E_1$

P $\equiv E_0$

We study this model in 2-site lattice : $i = 1$ & $i = 2$, and the number of electron $N = 2$. The Hilbert space has 6-states :

$\lvert\uparrow\uparrow\rangle = c^\dagger_{1\uparrow} c_{2\uparrow} \lvert 0\rangle$	—	$E_0 = -2\mu$	} P
$\lvert\uparrow\downarrow\rangle$	—	"	
$\lvert\downarrow\uparrow\rangle$	—	"	
$\lvert\downarrow\downarrow\rangle$		"	
$\lvert 2\,0\rangle$	...	$E_0 = -2\mu + V$	} Q
$\lvert 0\,2\rangle$		$E_0 = -2\mu + V$	

- So, we want an effective Hamiltonian that acts only on the four states $\in$ P and the remaining high energy doubly occupied states Q should be eliminated.

- For us the perturbation is

$$V = H_t = -t\left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)$$

Then

$\langle \uparrow\uparrow | V | \uparrow\uparrow \rangle = 0$ and the same for all the $\uparrow$ states.

$\langle 20 | V | \uparrow\uparrow \rangle = 0$ and the same for the $\downarrow$ spin, due to exclusion principle.

$\langle 20 | V | \uparrow\downarrow \rangle = +t$ (we get opposite sign because of normal ordering)

$\langle 02 | V | \uparrow\downarrow \rangle = -t$.

$\langle 20 | V | \downarrow\uparrow \rangle = -t$

$\langle 02 | V | \uparrow\downarrow \rangle = +t$.

Then $\langle \uparrow\downarrow | H_{eff} | \uparrow\downarrow \rangle = -2\mu - \frac{2t^2}{U}$.

$\langle \downarrow\uparrow | H_{eff} | \downarrow\uparrow \rangle = -2\mu - \frac{2t^2}{U}$.

$\langle \uparrow\downarrow | H_{eff} | \downarrow\uparrow \rangle = \frac{2t^2}{U}$.

$\langle \downarrow\uparrow | H_{eff} | \uparrow\downarrow \rangle = \frac{2t^2}{U}$.

we notice that we only have off diagonal terms for the $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ channel, i.e. for the $S=0$ channel, while $|\uparrow\uparrow\rangle$ & $|\downarrow\downarrow\rangle$ terms have no contribution from the interaction.

So, we write the 2×2 Heff Hamiltonian in the spinor of $(|\uparrow\downarrow\rangle \; |\downarrow\uparrow\rangle)^T$ as

$$H_{eff} = -2\mu\, \mathbb{I} + \frac{2t^2}{U}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$= \left(-2\mu - \frac{2t^2}{U}\right)\mathbb{I} + \frac{2t^2}{U}\sigma_x .$$

So, we simply have to go to the eigen basis of the σ_x, which is

$$\phi_+ = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad \phi_- = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$, for the eigenvalues of $\sigma_x = \pm 1$. Therefore, the eigen values of Heff is

$$E^{\pm} = -2\mu, \; -2\mu - \frac{4t^2}{U}.$$

and the corresponding eigen values are

$$\psi_+ = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \quad \text{"triplet"}$$
$$\psi_- = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad \text{singlet.}$$

In other words, the 4×4 Heff Hamiltonian has three triplet states which are degenerate at $E^+ = -2\mu$ and a singlet state at a lower energy $E^- = -2\mu - 4t^2/U$.

$$-2\mu \quad \text{---} \quad |\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \qquad S = 1$$

$$-2\mu - \frac{4t^2}{U} \quad \text{---} \quad \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \qquad S = 0.$$

- This is not very surprising, because, the effective Hamiltonian is symmetric under spin rotation of the system. So, the total spin ang momentum, $\vec{S} = \vec{S}_1 + \vec{S}_2$, commutes with Heff. Since $S = 0, 1$, so, the Hamiltonians eigenstate must have the same spin quantum number.

- Therefore, the 4×4 Hamiltonian can be written in the spin basis of two spin-1/2 particles as

$$H_{eff} = J\,\vec{S}_1 \cdot \vec{S}_2 - \mu \sum_{i=1,2,\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} \quad \text{--- (6a)}$$

where $\boxed{J = \frac{4t^2}{U}}$, called the super exchange term.

and. $\vec{S}_i = \frac{1}{2} \sum_{\alpha,\beta=\uparrow,\downarrow} c^{\dagger}_{i\alpha}\, \vec{\sigma}_{\alpha\beta}\, c_{i\beta}$.

- For the lattice of N- sites, the model is easily generalized

$$H_{eff} = J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j - \mu \sum_{i=1,\sigma}^{N} c^{\dagger}_{i\sigma} c_{i\sigma}.$$

This is the Heisenberg Hamiltonian, but with an additional chemical potential constraint that the total number of electrons must be conserved.

- As we move away from half-filling, and add or remove some electrons, the double occupancy states from the Q-manifold have to be accessed. For P to Q manifold are jumped or hopped by the H_t term, and hence we can add it to get

$$\boxed{H_{eff} = -t \sum_{\langle ij \rangle, \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^{\dagger}_{i\sigma} c_{i\sigma} + J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j}$$

— (6b)

This is the celebrated t-J model.

- Since $J = 4t^2/U > 0$, therefore, we get a negative energy contribution if the spins in neighboring sites are anti-parallel to each other, ie, $S_i = +\vec{S}_i$ and $\vec{S}_{i+1} = -\vec{S}_i$, that $S_i . S_i = -S_i^2 = -1/4$, which gives the total energy density as $E = -J\,1/4 = -t^2/U$, as also obtained in from the mean field theory of the Hubbard model.

- This model also has the spin liquid state, in which the singlet states between the nearest neighbors, remain disorder, rather than become ordered as in the AFM case. Usually ordering always lowers the energy, but to obtain disorder state at zero-temperature, one needs additional constraint such as lattice frustration. Once such a disorder state is obtained at zero temperature - we call it a spin liquid state. This is also known as the Resonating valence bond (RVB) state.
- The t-J model also has superconducting instability away from half-filling, which was originally proposed for the high-T_c copper oxide superconductors by G. Baskaran and P.W. Anderson. But experimentally, there is not much evidence of the RVB superconductivity in this compound, prompting the idea is that perhaps the Hubbard U is not that large, and one needs to starts from the weak coupling (Fermi liquid) limit.