

## Itinerant magnetism and the Hubbard model

In Fe, Co and Ni, magnetism comes from conduction electrons. This is what we call itinerant magnetism. The Hubbard model is the most important model in this context. It describes, besides itinerant magnetism, metal-insulator (Mott) transitions and even high temperature superconductivity.

soft stems with angular leaves with

leaves drooping

## Introduction

So far we have discussed only localized magnetism, meaning we were able to attribute a spin to each site in the lattice. This is not how things work in Fe, Ni and Co (the most important ferromagnetic elements) and many other compounds. In these cases, the magnetic electrons are actually the conduction electrons. This is what we call itinerant magnetism.

There is still a lot we don't know about itinerant magnetism. We just don't know how to write down the Hamiltonian. We usually have to resort to mean field approximations (in this context they are usually called Hartree-Fock approximation, but it's the same thing). For some materials mean field seems to work well. For others, it sometimes fails miserably. Systems for which mean-field fails are called strongly correlated.

The starting point is very simple. We have a system of  $N$  electrons in a box. The electrons feel a potential  $V(r)$  due to the ions, which we assume to remain fixed. They also repel each other due to the Coulomb interaction. Thus, the first quantized Hamiltonian will be

$$H = \sum_{i=1}^N \left\{ \frac{p_i^2}{2m} + V(r_i) \right\} + \frac{1}{2} \sum_{i \neq j} V(r_i - r_j) \quad (1)$$

where  $V(r) = e^2/r$  is the Coulomb potential.

We now move to second quantization. Recall that given any single-particle basis  $|x\rangle$ , we may write a single-particle Hamiltonian  $A$  as

$$A = \sum_{\alpha, \beta} \langle \alpha | A | \beta \rangle a_\alpha^\dagger a_\beta \quad (2)$$

and a 2-body operator  $V$  as

$$V = \frac{1}{2} \sum_{\alpha \beta \gamma \delta} \langle \alpha, \beta | V | \gamma, \delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \quad (3)$$

we could choose as basis the position kets  $|x\rangle$  or the momentum kets  $|k\rangle$ . But for what we are going to do, it is more convenient to choose the Wannier / tight-binding basis  $|i, \mu, \sigma\rangle$ , defined

as

$$|i, \mu, \sigma\rangle = \text{electron at position } i, \text{ orbital } \mu \text{ and} \\ \text{spin } \sigma = \uparrow, \downarrow \quad (4)$$

This is a complete basis. For more information, check out problem set 1, problems 3 and 4.

We can use the basis (4) to write down an exact 2<sup>nd</sup> quantized Hamiltonian. But since we can't solve it anyways, I will already start making some approximations. The first one is to assume that transitions between different orbitals are negligible.

This means we can neglect terms with transitions  $\sigma \rightarrow \sigma$ . Effectively, this means that the dynamics of the different orbitals factors out completely, so we can focus on just one orbital. Thus, I will henceforth write the basis (1) simply as  $|i, \sigma\rangle$ .

Returning now to the Hamiltonian (1) and using (2) and (3), we may write

$$H = - \sum_{ij\sigma} g_{ij} a_{i\sigma}^+ a_{j\sigma} + \frac{1}{2} \sum_{\substack{i,j \\ \sigma, \sigma'}} \delta(i_j, i'_j) a_{i\sigma}^+ a_{j\sigma} a_{i\sigma'} a_{j\sigma'}$$
(5)

where

$$g_{ij} = - \langle i | H_0 | j \rangle$$
(6)

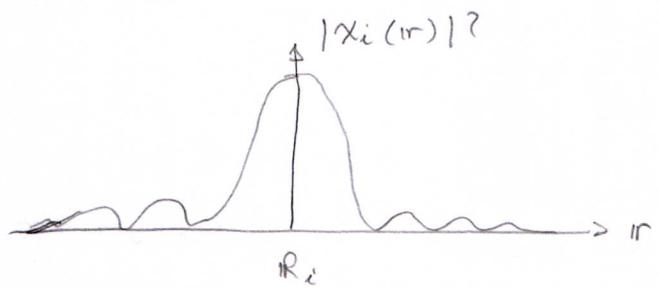
$$\delta(i_j, i'_j) = \langle i_j | V | i'_j \rangle$$

This Hamiltonian is still quite messy. The first term is the tight-binding term, which we know how to treat. But we must try to simplify the second term further. It is simply too messy.

To understand what it means, define the Wannier functions

$$X_i(r) = \langle i | r \rangle \quad (7)$$

Recall that this function is localized at site  $R_i$



The matrix elements  $\delta(ij, i'j')$  then become

$$\delta(ij, i'j') = \int dx dy \ X_i(x) X_j(y) V(x-y) X_{i'}(x) X_{j'}(y) \quad (8)$$

This means we are talking about the overlap of Wannier functions of 4 different sites, weighted by  $V(x-y)$ . Since the Wannier functions are highly localized, we expect this overlap to be significant only for close by sites and specially for the same site

In his original paper, Hubbard gave the following estimate for Ni:

$$\sigma(ii, ii) \approx 20 \text{ eV}$$

$$\sigma(ij, ij) \approx 6 \text{ eV}$$

$$\sigma(ii, ij) \approx 0.5 \text{ eV}$$

$$\sigma(ij, ik) \approx 0.5 \text{ eV}$$

$$\sigma(ij, ji) = 0.025 \text{ eV}$$

$$\sigma(ii, jj) \approx 0.025 \text{ eV}$$

$i, j, k$  nearest  
neighbors

thus, we see that the dominant contribution comes from the on-site repulsion.

If we consider only this form we obtain the Hubbard model

$$g_L = - \sum_{ij\sigma} g_{ij\sigma} a_{i\sigma}^+ a_{j\sigma}^- + \frac{U}{2} \sum_{i,j,\sigma} a_{i\sigma}^+ a_{i\sigma}^+ a_{j\sigma}^- a_{j\sigma}^-$$

where  $U = \sigma(ii, ii)$ . Now, due to the Pauli principle,  $(a_{i\sigma}^+)^2 = (a_{i\sigma}^-)^2 = 0$  so in the last form we only need to consider the  $\delta$  terms which are opposite from  $\sigma$ .

Thus we write it as

$$\frac{U}{2} \sum_{i\sigma} a_{i\sigma}^+ a_{i\bar{\sigma}} + a_{i\bar{\sigma}}^+ a_{i\sigma}$$

where  $\bar{\sigma} = -\sigma$  (just a more convenient way of writing it).

We may further manipulate this as

$$\begin{aligned} a_{i\sigma}^+ a_{i\bar{\sigma}}^+ a_{i\bar{\sigma}} a_{i\sigma} &= -a_{i\sigma}^+ a_{i\bar{\sigma}}^+ a_{i\bar{\sigma}} a_{i\sigma} \\ &\quad \xrightarrow{-1} \quad \xrightarrow{-1} \\ &= a_{i\sigma}^+ a_{i\bar{\sigma}} a_{i\bar{\sigma}}^+ a_{i\bar{\sigma}} \end{aligned}$$

thus, we see here the number operators  $\hat{n}_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$ .  
we therefore may finally write the Hubbard Hamiltonian

as

$$H = - \sum_{ij\sigma} g_{ij} a_{i\sigma}^+ a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}}$$

(9)

Previously we studied the Base-Hubbard model. Here the last term gave an extra energy when a site was more than doubly occupied. For Fermions the only way a site can be more than doubly occupied is by having one electron with spin up and the other with spin down.

Let me make some comments about the Hubbard model. First, we neglected from the start the possibility of having multiple orbitals per site. If we had excluded that, the last form in (5) would have to be replaced by

$$\sigma(i\mu j\nu; i'\mu' j'\nu')$$

If  $x_{i\mu}$  is the Wannier function corresponding to an electron at orbital  $\mu$  of site  $i$ , then

$$\sigma(i\mu j\nu; i'\mu' j'\nu') = \int d^3x d^3y x_{i\mu}(x) x_{j\nu}(y) v(x-y) x_{i'\mu'}(x) x_{j'\nu'}(y)$$

now we have all sorts of repulsions between orbitals in the different bands. The most important contribution still comes from the same sites

$$\sigma(\mu\nu; \mu'\nu') = \sigma(i\mu i\nu; i\mu' i\nu')$$

$$= \int d^3x d^3y x_{i\mu}(x) x_{i\nu}(y) v(x-y) x_{i\mu'}(x) x_{i\nu'}(y)$$

But now we have a bunch of orbital repulsions.

The most important terms are the direct terms

$$\text{Direct: } \mu' = \mu, \nu' = \nu \Rightarrow \delta(\mu\nu, \mu\nu)$$

and the exchange term

$$\text{Exchange: } \mu' = \nu, \nu' = \mu \Rightarrow \delta(\mu\nu, \nu\mu)$$

Let us also recall the basic properties of the Hubbard model

- One orbital per atom
- On-site repulsion only
- One atom per unit cell

The properties of the Hubbard model will be dictated by 4 main properties

1) on-site repulsion  $\delta$

2) Tight-binding hopping rate and bandwidth

3) Filling  $\rho = \frac{1}{N} \sum_{i\sigma} \langle n_{i\sigma} \rangle \quad (0 \leq \rho \leq 2)$

4) Crystal structure and dimensionality

## the Stomer mean-field approximation

the first attempt at any many-body Hamiltonian in a mean-field approximation. we write, as always,

$$\hat{m}_{i\sigma} = \langle \hat{m}_{i\sigma} \rangle + (\hat{m}_{i\sigma} - \langle \hat{m}_{i\sigma} \rangle) \quad (10)$$

Due to translation invariance we must have

(11)

$$\langle \hat{m}_{i\sigma} \rangle = m_\sigma$$

Thus

$$\hat{m}_{i\sigma} = m_\sigma + (\hat{m}_{i\sigma} - m_\sigma)$$

We now insert this in the last term of (9);

$$\begin{aligned} \sum_{i\sigma} m_{i\sigma} \hat{m}_{i\bar{\sigma}} &= \sum_{i\sigma} [m_\sigma + (\hat{m}_{i\sigma} - m_\sigma)] [\bar{m}_\sigma + (\hat{m}_{i\bar{\sigma}} - \bar{m}_\sigma)] \\ &= \sum_{i\sigma} [m_\sigma \bar{m}_\sigma + m_\sigma (\hat{m}_{i\bar{\sigma}} - \bar{m}_\sigma) + \bar{m}_\sigma (\hat{m}_{i\sigma} - m_\sigma) \\ &\quad + O(\text{fluctuations squared})] \end{aligned}$$

$$\approx -2N m_\sigma \bar{m}_\sigma + \sum_{i\sigma} (m_\sigma \hat{m}_{i\bar{\sigma}} + \bar{m}_\sigma \hat{m}_{i\sigma})$$

$$= -2N m_\sigma \bar{m}_\sigma + 2 \sum_{i\sigma} \hat{m}_{i\sigma} \hat{m}_{i\bar{\sigma}}$$

(9)

thus, the Hubbard Hamiltonian (9) is approximated to

$$H \approx - \sum_{ij\sigma} g_{ij} a_{i\sigma}^+ a_{j\sigma} + U \sum_{i\sigma} \hat{n}_{i\sigma} n_{i\sigma} + \text{const} \quad (12)$$

Now we move to Fourier space

$$a_{i\sigma}^+ = \frac{1}{\sqrt{N}} \sum_k e^{ikR_i} a_{k\sigma}^+ \quad (13)$$

Recall that the Fourier transformation does not affect the total number of particles

$$\sum_{i\sigma} \hat{n}_{i\sigma} = \sum_{i\sigma} a_{i\sigma}^+ a_{i\sigma} = \sum_{k\sigma} a_{k\sigma}^+ a_{k\sigma} \quad (14)$$

Moreover, we know that moving to Fourier space diagonalizes the tight-binding part

$$- \sum_{ij\sigma} g_{ij} a_{i\sigma}^+ a_{j\sigma} = \sum_{k\sigma} \epsilon_k a_{k\sigma}^+ a_{k\sigma} \quad (15)$$

thus, eq (12) becomes

$$H = \sum_{k\sigma} \epsilon_{k\sigma} a_{k\sigma}^+ a_{k\sigma}, \quad \epsilon_{k\sigma} = \epsilon_k + Un \quad (16)$$

## Thermal properties and phase transition

The quantities  $m_\sigma$  in Eq (16) must now be determined self-consistently. We know from statistical mechanics that

$$\langle a_{\sigma \omega}^+ a_{\sigma \omega} \rangle = \frac{1}{e^{\beta(E_{\sigma \omega} - \mu)} + 1} \quad (17)$$

Thus, the total number of particles with spin  $\sigma$  will be

$$\sum_m \langle a_{\sigma \omega}^+ a_{\sigma \omega} \rangle = \sum_m \frac{1}{e^{\beta(E_{\sigma \omega} - \mu)} + 1} \quad (18)$$

But this must be  $N_\sigma$  where, recall,  $N$  is the number of sites. Thus we get the self-consistency equation

$$N_\sigma = \frac{1}{N} \sum_m \frac{1}{e^{\beta(E_{\sigma \omega} - \mu)} + 1} \quad (19)$$

These are actually two equations which must be solved for  $m_\uparrow$  and  $m_\downarrow$ .

Define the density of states as extremer element

$$\frac{1}{N} \sum_{\text{all}} f(\epsilon_n) = \int_{-\infty}^{\infty} d\epsilon D(\epsilon) f(\epsilon)$$

where I include the  $1/N$  in the definition just for convenience. then we get

$$m_0 = \int d\epsilon \frac{D(\epsilon)}{e^{(E+UM\bar{f}-\mu)/kT} + 1} \quad (20)$$

Now define

$$\begin{aligned} m &= m_{\uparrow} - m_{\downarrow} \\ p &= m_{\uparrow} + m_{\downarrow} \end{aligned} \quad (21)$$

Inverting

$$\begin{aligned} m_{\uparrow} &= \frac{p+m}{2} \\ m_{\downarrow} &= \frac{p-m}{2} \end{aligned} \quad (22)$$

Thus we get

$$n_F = \int d\epsilon \frac{D(\epsilon)}{e^{\beta(\epsilon + \frac{U_F}{2} - \mu)} + 1} \quad (23)$$

$$n_B = \int d\epsilon \frac{D(\epsilon)}{e^{\beta(\epsilon + \frac{U_F}{2} + \frac{U_M}{2} - \mu)} + 1}$$

combining these two equations we get

$$\rho = \int d\epsilon D(\epsilon) \left\{ \frac{1}{e^{\beta(\epsilon + \frac{U_F}{2} - \frac{U_M}{2} - \mu)} + 1} + \frac{1}{e^{\beta(\epsilon + \frac{U_F}{2} + \frac{U_M}{2} - \mu)} + 1} \right\} \quad (24)$$

$$m = \int d\epsilon D(\epsilon) \left\{ \frac{1}{e^{\beta(\epsilon + \frac{U_F}{2} - \frac{U_M}{2} - \mu)} + 1} - \frac{1}{e^{\beta(\epsilon + \frac{U_F}{2} + \frac{U_M}{2} - \mu)} + 1} \right\}$$

the first one is actually an equation for  $\rho(\rho, m)$ , since  $\rho$  is the quantity fixed experimentally.

We may also rewrite the equation for  $m$  as

$$m = \tanh\left(\frac{\beta U_M}{2}\right) \int d\epsilon \frac{D(\epsilon)}{\cosh(\beta(\epsilon + \frac{U_F}{2} - \mu)) + \cosh(\frac{\beta U_M}{2})} \quad (25)$$

Let us analyze the low temperature behavior. If  $m \approx 0$  then the chemical potential will be

$$\mu \approx \epsilon_F + \frac{U_f}{2} \quad (26)$$

where  $\epsilon_F$  is the Fermi level of the tight-binding system when  $U=0$ . Then Eq (25) becomes

$$m \approx \tanh\left(\frac{\beta U m}{2}\right) \int d\epsilon \frac{D(\epsilon)}{\cosh(\beta(\epsilon - \epsilon_F)) + \cosh\left(\frac{\beta U m}{2}\right)} \quad (27)$$

close to the critical point,  $m$  will be small and we may thus expand

$$\tanh\left(\frac{\beta U m}{2}\right) \approx \frac{\beta U m}{2}$$

$$\cosh\left(\frac{\beta U m}{2}\right) \approx 1$$

This defines the wave temperature  $T_c$  according to

$$T_c = \frac{U}{2} \int d\epsilon \frac{\beta_c D(\epsilon)}{\cosh(\beta_c(\epsilon - \epsilon_F)) + 1} \quad (28)$$

To solve for  $T_c$  we need to know the density of states  $D(\epsilon)$ . But before we do so, we must first ask whether there will be a transition or not. In the worst case scenario, the transition should occur at  $T_c = 0$  ( $\beta_c = \infty$ ). In this limit we may use the following convenient representation of the  $f$  function

$$f(x) = \lim_{\beta \rightarrow \infty} \frac{1}{2} \frac{\beta}{1 + \cosh(\beta x)} \quad (29)$$

Using this in (28) then gives

$$\begin{aligned} I &= U \int d\epsilon D(\epsilon) f(\epsilon - \epsilon_F) \\ &= U D(\epsilon_F) \end{aligned}$$

Thus, if the transition is to exist, we must have

$$UD(\epsilon_F) \geq I \quad (30)$$

This is called the Stover criterion. It is the condition that must be satisfied for a transition to exist.

This actually makes some sense if we look at the transition metals

- In a row of the transition metals, in the periodic table, the number of conduction electrons increases from left to right so  $D(\epsilon_F)$  increases
- In a column, the total number of electrons increases from top to bottom, increasing the Coulomb screening and hence decreasing  $\sigma$

thus, the Stoner criterion should be satisfied in the upper right corner, which is exactly where Fe, Co and Ni are.

As another example, suppose  $D(\epsilon)$  is actually flat within a certain band width

$$D(\epsilon) = \begin{cases} \frac{1}{w} & \text{if } \epsilon \in [-\frac{w}{2}, \frac{w}{2}] \\ 0 & \text{otherwise} \end{cases} \quad (31)$$

then Eq (28) gives

$$I = \frac{\beta_C U}{2} \frac{1}{w} \int_{-w/2}^{w/2} d\epsilon \frac{1}{\cosh(\beta_C(\epsilon - \epsilon_F)) + 1}$$

$$I = \frac{U}{2w} \left\{ \tanh\left(\frac{\beta_C}{2}\left(\frac{w}{2} - \epsilon_F\right)\right) - \tanh\left(\frac{\beta_C}{2}\left(-\frac{w}{2} - \epsilon_F\right)\right) \right\}$$

We see that  $\beta_C$  will depend on  $\epsilon_F$ , which is a function of the filling  $\rho$ .

Suppose  $\epsilon_F = 0$  (half filling). Then

$$\frac{w}{U} = \tanh\left(\frac{\beta_C w}{4}\right)$$

$$\frac{\beta_C w}{4} = \tanh^{-1}(w/U)$$

or

or

$$T_C = \frac{w}{4} \frac{1}{\tanh^{-1}(w/U)}$$

Let's make a crude estimate. Usually  $w$  (the band width) is in the interval 1-10 eV and  $U$  is in the interval 2-20 eV. When  $w/U < 0.5$  we may approximate  $\tanh^{-1}(w/U) \approx w/U$ . Thus we get

$$T_c \approx \frac{U}{4} \quad (32)$$

Recall that 300 K is 0.026 eV. So, since  $U=2-20$  eV, this would imply

$$T_c \approx 10^9 \text{ K}$$

which is absurd. Thus we conclude that the Stoner mean field approximation clearly overestimates  $T_c$ . This is true of most mean-field approximations.

## Antiferromagnetism at half-filling

In the limit  $U/g \rightarrow \infty$  the system becomes localized in the Mott phase. Now I want to show that when  $U/t$  is large but finite, the Hubbard model gives rise to an antiferromagnetic Heisenberg interaction, exactly at  $\frac{1}{2}$  filling ( $P=1$ )

It suffices to consider two sites only. The Hubbard Hamiltonian then becomes

$$(33) \quad H = H_U + H_g$$

where

$$(34) \quad H_U = \frac{U}{2} \sum_{\sigma} \left( \hat{m}_{1\sigma} \hat{m}_{1\bar{\sigma}} + \hat{m}_{2\sigma} \hat{m}_{2\bar{\sigma}} \right)$$

$$= U \left( \hat{m}_1^+ \hat{m}_1^- + \hat{m}_2^+ \hat{m}_2^- \right)$$

$$(35) \quad H_g = -g \sum_{\sigma} (a_{1\sigma}^\dagger a_{2\sigma} + a_{2\sigma}^\dagger a_{1\sigma})$$

We assume  $U \gg g$  so that  $H_g$  may be treated as a perturbation.

Now we use a lovely trick based on a similarity transformation.

Consider the following Hamiltonian transformation. Consider the following Hamiltonian

$$(36) \quad H' = e^{g\hat{\theta}} H e^{-g\hat{\theta}}$$

where  $\hat{\theta}$  is some operator.

The Hamiltonian  $H'$  has the same eigenvalues of  $H$ . For, if  $H|m\rangle = E_m|m\rangle$  then

$$H|m\rangle = e^{-g\hat{\theta}} H' e^{g\hat{\theta}} |m\rangle = E_m|m\rangle$$

Thus

$$H' \left[ e^{g\hat{\theta}} |m\rangle \right] = E_m \left[ e^{g\hat{\theta}} |m\rangle \right] \quad (37)$$

the eigenvalues are thus the same as those of  $E_m$ , whereas the eigenvectors get multiplied by  $e^{g\hat{\theta}}$ .

Back to (36), we now use the BCH formula to rewrite

$$H' = e^{g\hat{\theta}} H e^{-g\hat{\theta}} = H + g [\hat{\theta}, H] + \frac{g^2}{2} [\hat{\theta}, [\hat{\theta}, H]] + \dots \quad (38)$$

We use this to make a sort of perturbation theory in the parameter  $g/v$ . Let us write (38) as

$$\begin{aligned} H' &= H_0 + H_g + g [\hat{\theta}, H_0] + g [\hat{\theta}, H_g] + \\ &\quad + \frac{g^2}{2} [\hat{\theta}, [\hat{\theta}, H_0]] + \frac{g^2}{2} [\hat{\theta}, [\hat{\theta}, H_g]] + \dots \end{aligned} \quad (39)$$

Now we choose  $\hat{\theta}$  so as to eliminate all terms linear in  $g$ . That is, such that

$$\boxed{H_g + g [\hat{\theta}, H_0] = 0} \quad (40)$$

thus we get

$$H' = H_0 + g [\sigma, Hg] + \frac{g^2}{2} [\sigma, [\sigma, H_0]] + \sigma(g)^3 \quad (41)$$

I like this method: it's a way of doing perturbation theory in the level of operators instead of states

Now we need to solve the operator Eq (40) for  $\sigma$ . Recall that we want to work at 1/2 filling,  $\rho=1$ . This means that out of the 4 possible states (two for each site), we will always have two occupied. Our Hilbert space will therefore be described by the subspace

$$\begin{aligned} |S_1\rangle &= a_{1\uparrow}^\dagger a_{2\uparrow}^\dagger |0\rangle \\ |S_2\rangle &= a_{2\uparrow}^\dagger a_{1\uparrow}^\dagger |0\rangle \\ |S_3\rangle &= a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle \\ |S_4\rangle &= a_{1\downarrow}^\dagger a_{2\downarrow}^\dagger |0\rangle \\ |D_1\rangle &= a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger |0\rangle \\ |D_2\rangle &= a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger |0\rangle \end{aligned} \quad (42)$$

where "S" stands for singly occupied and "D" for doubly occupied. Define also the projection operators

$$P_S = \sum_{i=1}^4 |S_i\rangle \langle S_i| \quad (43)$$

$$P_D = \sum_{i=1}^2 |D_i\rangle \langle D_i|$$

they project onto the singly and doubly occupied subspaces  
and they satisfy all properties of projection operators

$$\begin{aligned} P_s^2 &= P_s & P_d^2 &= P_d \\ P_s P_d &= P_d P_s = 0 \\ P_d + P_s &= I \\ P^\dagger &= P \end{aligned} \tag{44}$$

Now we write

$$\Theta = I \Theta I = (P_s + P_d) \Theta (P_s + P_d)$$

$$= P_s \Theta P_s + P_d \Theta P_d + P_s \Theta P_d + P_d \Theta P_s \tag{45}$$

The reason why I do this is because  $H_U$  only acts on  
doubly occupied states so

$$H_U P_s = P_s H_U = 0 \tag{46}$$

Moreover

$$H_U P_d = P_d H_U = 0 \tag{47}$$

Thus

$$\begin{aligned} [\Theta, H_U] &= \Theta H_U - H_U \Theta \\ &= U \{ P_d U P_d + P_s \Theta P_d - P_d \Theta P_d - P_d \Theta P_s \} \\ &= U \{ P_s \Theta P_d - P_d \Theta P_s \} \end{aligned}$$

Plugging this in (40) then gives the equation

$$P_s \otimes P_d - P_d \otimes P_s = -\frac{1}{g_0} Hg \quad (47)$$

Now multiply by  $P_d \dots P_s$ . The first term is zero due to (44) so we get

$$P_d \otimes P_s = \frac{1}{g_0} P_d Hg P_s$$

Similarly, multiply by  $P_s \dots P_d$ . We then get

$$P_s \otimes P_d = -\frac{1}{g_0} P_s Hg P_d$$

Thus, combining the two we conclude that

$$\boxed{\theta = \frac{1}{g_0} \{ P_d Hg P_s - P_s Hg P_d \}} \quad (48)$$

Now that we have this result we can go back to (41). we can also use in the last term that  $[\theta, H_0] = -\frac{Hg}{g_0}$ . We then get

$$H' = H_0 + g [\theta, Hg] - \frac{g}{2} [\theta, Hg]$$

$$\Rightarrow H' = H_0 + \frac{g}{2} [\theta, Hg] \quad (49)$$

or, explicitly,

$$H' = H_0 + \frac{1}{20} \left\{ P_d H_g P_s H_g - P_s H_g P_d H_g + \right. \\ \left. - H_g P_d H_g P_s + H_g P_s H_g P_d \right\}$$

Finally, let us analyze  $H'$  within the singly occupied subspace. Since  $P_s H_0 P_s = 0$  we get

$$P_s H' P_s = \frac{1}{20} \left\{ 0 - P_s H_g P_d H_g P_s + \right. \\ \left. - P_s H_g P_d H_g P_s + 0 \right\}$$

or

$$P_s H' P_s = -\frac{1}{20} (P_s H_g P_d H_g P_s + P_s H_g P_d H_g P_s) \quad (50)$$

we may also write this as

$$P_s H' P_s = -\frac{1}{10} P_s (H_g P_d H_g) P_s \quad (50)$$

Now, to finish, we need to figure out the meaning of this result!

Let us compute the matrix elements of (50) in the basis  $|S_i\rangle$ . We have

$$\langle S_i | H | S_j \rangle = -\frac{1}{U} \langle S_i | H_g P_d H_g | S_j \rangle$$

This is easily done numerically. we find, within this subspace

$$H' = \frac{2g^2}{U} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (51)$$

This looks identical to the Hamiltonian of two spin  $\frac{1}{2}$  particles

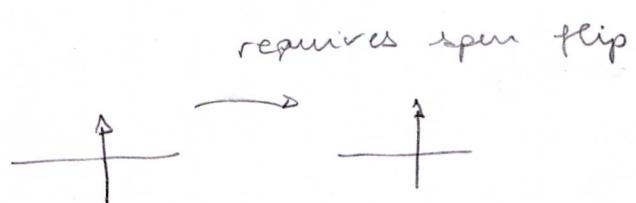
$$H = \frac{J}{4} (\vec{\sigma}_1 \cdot \vec{\sigma}_2 - 1) \quad (52)$$

where

$$J = \frac{4g^2}{U} \quad (53)$$

thus, we conclude that if restrict the problem to  $\frac{1}{2}$  filling, singly occupied dynamics and large  $U/g$ , we obtain an anti-ferromagnetic interaction between the electrons

The physics of this is the following. If two spins are parallel, they can only rearrange if there is a spin flip



But if they are anti-parallel, then they can hybridize and participate in an effective interaction



This mechanism was discovered by Anderson, which named it superexchange