Topic: Fermi Hubbard model

* We know the Hubbard model
* We can derive the Mott transition
* We know how to obtain an antiferromagnet.

0. Repetition

Given a periodic potential $V(\vec{r}) = \frac{I(r)}{\Delta}$

with $I(r) = \frac{\omega_L}{2\pi} \int_0^{2\pi/\omega_L} dt \, |E(r,t)|^2$; $\Delta = \omega_0 - \omega_L$

we want to obtain a Lattice Hamiltonian

$$H_0 = -t \sum_{\langle i,j \rangle, \sigma} \left[c_{i\sigma}^\dagger c_{j\sigma} + H.c. \right].$$

(i) solve $\left\{ -\frac{\hbar^2}{2m} \left[\partial_x^2 + \partial_y^2 + \partial_z^2 \right] + V(\vec{r}) \right\} \psi(\vec{r}) = E \psi(\vec{r})$

(ii) Bloch theorem $\psi_{n,q} = e^{i\vec{q}\vec{r}} \sum_m a_{nq}^m e^{i\vec{K}_m \vec{r}}$

(iii) $w_{i,n}(\vec{r}) = w_n(\vec{r} + \vec{r}_i) = \int \frac{dq}{2\pi} \psi_{n,q} \, e^{i\vec{q}\vec{r}_i}$

$\Rightarrow$ $w_{i,n}(\vec{r})$: Wannier functions are centered on $\vec{r}_i$, are orthogonal, and fall off exponentially.

$$\Rightarrow \int d\vec{r}\, \hat{\psi}^{\dagger}(\vec{r}) \left[-\frac{\hbar^2}{2m} \vec{\nabla}^2 + V(\vec{r}) \right] \hat{\psi}(\vec{r}) = \sum_{\substack{ij \\ n,m}} c_{in}^{\dagger} c_{jm} \int d\vec{r}\, w_{in}^{*}(\vec{r}) \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\vec{r}) \right] w_{jm}(\vec{r})$$

$$\approx -t \sum_{\langle ij \rangle} c_{in}^{\dagger} c_{jn}$$

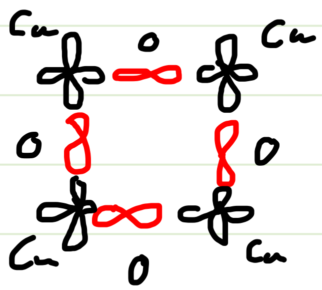
If we now also take interactions into account:

$$H = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}$$

with $U = \frac{4\pi\hbar^2 a_s}{m} \int d\vec{r}\, |w(\vec{r})|^4$.

This model is the simplest Hamiltonian for interacting fermions on a lattice. Despite its simplicity do we still have no clear understanding of its ground state. Before we continue we want to understand why it is so central in solid state research.

2. The cuprates



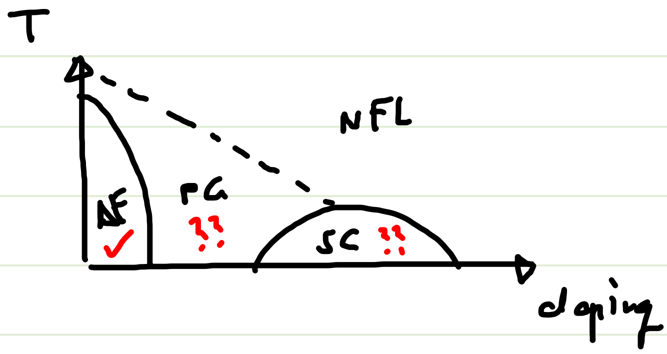
$LaCuO_4$

$\downarrow$

$3d^{10} 4s^1$

$\downarrow$

Cu^{2+} $3d^9$ $\Rightarrow$ one hole per Cu



3.) The Mott transition

We want to understand how to describe the large-U phases. This is complicated due to the four operators in $c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{i\downarrow} c_{i\downarrow}$. Let us try to find an approximate method.

One way to go is to try to cast $c^\dagger c c^\dagger c$ into something "quadratic".

Slave-spins: We double the degrees of freedom. Then we get rid of them via a constraint. The hope: at an intermediate stage, we have a simpler problem.

$$c^\dagger_{i\sigma} = 2 I^x_i f^\dagger_{i\sigma}$$

$$\{f_{i\sigma}, f^\dagger_{j\sigma'}\} = \delta_{ij}\delta_{\sigma\sigma'}$$

$$\{f_{i\sigma}, f_{j\sigma'}\} = \{f^\dagger_{i\sigma}, f^\dagger_{j\sigma'}\} = 0$$

$\vec{I}$: quantum spin-$\frac{1}{2}$

$$\Rightarrow \quad |0\rangle = |\Uparrow, 0\rangle \qquad |\uparrow\rangle = |\Downarrow, \uparrow\rangle$$

$$|\uparrow\downarrow\rangle = |\Uparrow, \uparrow\downarrow\rangle \qquad |\downarrow\rangle = |\Downarrow, \downarrow\rangle$$

$$\Rightarrow \quad I^z + \frac{1}{2} - (n_i - 1)^2 \equiv 0 \quad (1) \qquad n_i = n_{i\uparrow} + n_{i\downarrow}$$

Now, we can use this constraint to rewrite the interaction:

$$U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{U}{2} \sum_i n_i = \frac{U}{2} \sum_i (n_i - 1)^2 = \frac{U}{2} \sum_i \left(I_i^z + \frac{1}{2} \right)$$

$\Rightarrow$ U becomes a "simple" magnetic field for the slave spins!

For the kinetic term we get:

$$-4t \sum_{\langle ij \rangle \sigma} I_i^x I_j^x f_{i\sigma}^\dagger f_{j\sigma} .$$

$\Rightarrow$ this is a bit more troublesome: (i) Four operators, (ii) entangles "I" and "f" sector: each time an f-particle is hopping, also two slave spins are flipped.... (iii) We should keep track of all of these things as (1) has to be fulfilled.

$\Rightarrow$ We approximate by assuming that these sectors are <u>not entangled</u>

$$|\psi_{gs}\rangle = |\psi_F\rangle \otimes |\psi_I\rangle$$

$\Rightarrow \langle \psi_{gs} | H | \psi_{gs} \rangle$:

a.) $- t g \sum_{\langle ij \rangle \sigma} f_{i\sigma}^{\dagger} f_{j\sigma}$

b.) $- \chi t \sum_{\langle ij \rangle} I_i^x I_j^x + \frac{U}{2} \sum_i I_i^z$

with $g = 4 \langle I_i^x I_j^x \rangle$; $\chi = 4 \sum_\sigma [\langle f_{i\sigma}^{\dagger} f_{j\sigma} \rangle + \text{h.c.}]$

$\Rightarrow$ χ is just a number independent of t, U:

$$U_c = t\chi \sum_{\langle ij \rangle} = 16 \int_{-\infty}^{\varepsilon_F} d\varepsilon\, \varepsilon \rho_\sigma(\varepsilon) \approx 2.67\, t$$

$\Rightarrow$ How do we solve the spin model? Molecular-field:

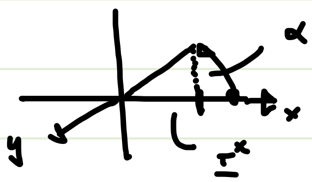
$$-\chi t \sum_{\langle ij \rangle} I_i^x I_j^x \approx -\chi t \langle I^x \rangle z \sum_i I_i^x$$

$$\Rightarrow \quad H_I = \vec{h} \sum_i \vec{I}_i \quad \text{with} \quad \vec{h} = \left(-\chi t \langle I^x \rangle, 0, \frac{U}{2}\right)$$

$$\Rightarrow \quad H_I = \frac{U_c}{2} \sqrt{u^2 + 4\langle I^x \rangle^2} \cdot \sum_i \tilde{I}^z_i \qquad u = \frac{U}{U_c}$$

with

$$\tilde{\vec{I}}_i = e^{i\alpha I^y_i} \vec{I}_i \, e^{-i\alpha I^y} \quad \text{with} \quad \tan\alpha = \frac{2\langle I^x_0 \rangle}{u}$$



$$\Rightarrow \quad \langle I^x \rangle = \frac{\sqrt{1-u^2}}{2}$$

$$\Rightarrow 4\langle I^x_i I^y_1 \rangle = \begin{cases} 1-u^2 \\ 0 \end{cases}$$

$$\Rightarrow \quad t_{eff}: \quad t \rightsquigarrow 0 \; ; \quad m: \quad m \rightsquigarrow \infty$$

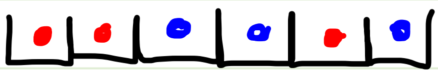
localization

Or the double occupancy:

$$d^2 = \frac{1}{2}\left(\langle I^z \rangle + \frac{1}{2}\right) = \begin{cases} \frac{1-u}{4} \\ 0 \end{cases}$$

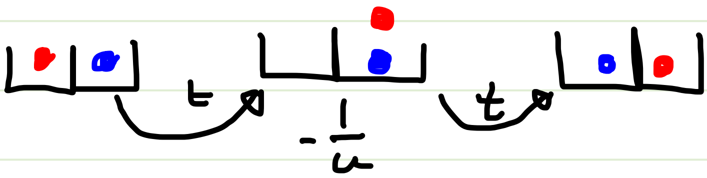
4. Spin-physics.

We know: $U > U_c$: $m^* \to \infty$, $d \to 0$



$\Rightarrow$ Is there any residual energy for spin-ordering?

Let us do 2^{nd} order perturbation theory



$\Rightarrow J \sim \frac{t^2}{U}$

but: only active if no two spins of the same flavor are next to each other!

$$\Rightarrow H = J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j$$

which we derive in the exercises.