Phys 506 lecture 38: Hubbard model

1 Original Mott picture

Consider a collection of H atoms. As we bring the atoms together they will solidify into a solid lattice (ignoring any molecular bonding effects for the moment).

When in a solid form, the 1s electrons spread into an energy band and there is one electron per lattice site.

This can be described by a tight-binding model for the 1s electrons, which allows electrons to "hop" between nearest neighbors.

$$\hat{T} = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma})$$

where $\langle ij \rangle$ counts nearest neighbors once. Because the electrons are negatively charged, we also expect Coulomb repulsion. But because the electrons are mobile, and can screen each other out, we approximate the repulsion by an on-site U only:

$$\hat{U} = U \sum_i n_{i\uparrow} n_{i\downarrow}.$$

The Hubbard model is the sum of these two terms

$$\boxed{\hat{H}_{\text{Hubbard}} = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow}.}$$

2 Momentum-space Hamiltonian

Let's examine $\hat{H}$ in momentum space (Bloch basis). Define:

$$a^\dagger_{k\sigma} = \frac{1}{\sqrt{V}} \sum_j e^{ik\cdot r_j} c^\dagger_{j\sigma}$$

$$a_{k\sigma} = \frac{1}{\sqrt{V}} \sum_j e^{-ik\cdot r_j} c_{j\sigma}$$

where V is the number of lattice sites. Then,

$$c^\dagger_{j\sigma} = \frac{1}{\sqrt{V}} \sum_k e^{-ik\cdot r_j} a^\dagger_{k\sigma}$$

$$c_{j\sigma} = \frac{1}{\sqrt{V}} \sum_k e^{ik\cdot r_j} a_{k\sigma},$$

which we can plug into the Hubbard Hamiltonian.

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \frac{1}{V} \sum_{kk'} \left(e^{-ik\cdot r_i + ik'\cdot r_j} a^\dagger_{k\sigma} a_{k'\sigma} + e^{ik\cdot r_i - ik'\cdot r_j} a^\dagger_{k'\sigma} a_{k\sigma} \right)$$
$$+ U \sum_i \frac{1}{V^2} \sum_{k_1,k_2,k_3,k_4} e^{-i(k_1-k_2)\cdot r_i - i(k_3-k_4)\cdot r_i} a^\dagger_{k_1\uparrow} a_{k_2\uparrow} a^\dagger_{k_3\downarrow} a_{k_4\downarrow}.$$

Note that for nearest neighbor pairs $r_j = r_i + \delta$ with δ being the nearest neighbor translation vector. So,

$$\frac{1}{V} \sum_{\langle ij \rangle} e^{-ik\cdot r_i + ik'\cdot r_j} = \frac{1}{V} \frac{1}{2} \sum_i \sum_\delta e^{-i(k-k')\cdot r_i + ik'\cdot\delta}$$
$$= \frac{1}{2} \sum_\delta e^{ik\cdot\delta} \delta_{kk'}.$$

So the first term (kinetic energy) becomes $\sum_{k\sigma} = \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma}$ with

$$\varepsilon_k = -t \frac{1}{2} \sum_\delta (e^{ik\cdot\delta} + e^{-ik\cdot\delta}) = -t \sum_\delta \cos(k\cdot\delta)$$

and the second term becomes

$$\frac{U}{V} \sum_{kk'q} a^\dagger_{k+q\uparrow} a_{k\uparrow} a^\dagger_{k'-q\downarrow} a_{k'\downarrow}.$$

So we find that the Hubbard Hamiltonian takes the following form in momentum space:

$$\hat{H} = \sum_{k\sigma} = \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} + \frac{U}{V} \sum_{kk'q} a^\dagger_{k+q\uparrow} a_{k\uparrow} a^\dagger_{k'-q\downarrow} a_{k'\downarrow}.$$

Note that in real space the first term is complicated but the second term is diagonal, while the opposite occurs in momentum space. The key problem is to find the eigenvalues and properties of the ground state for arbitrary U values.

3 Symmetries of the Hubbard model

Suppose the lattice is bipartite $\implies$ $t_{ij} \neq 0$ only if $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$ (never AA or BB). Some examples with nearest neighbor hopping:

- Simple cubic lattice
- Square lattice
- Body-centered cubic lattice
- NOT face-centered cubic lattice
- NOT triangular lattice

Then, $t \to -t$ is a symmetry.

Proof: Define $(c'_{i\sigma})^\dagger = (-1)^{\varepsilon(i)} c^\dagger_{i\sigma}$ and $c'_{i\sigma} = (-1)^{\varepsilon(i)} c_{i\sigma}$ with $\varepsilon(i) = 1$ when $i \in A$ and 0 when $i \in B$. Then,

$$\hat{H} = t \sum_{\langle ij\rangle\sigma} ((c'_{i\sigma})^\dagger c'_{j\sigma} (c'_{j\sigma})^\dagger c'_{i\sigma}) + U \sum_i n'_{i\uparrow} n'_{i\downarrow}$$

since $c^\dagger_{i\sigma} c_{j\sigma} = -(c'_{i\sigma})^\dagger c'_{j\sigma}$ when i and j are on different sublattices. Therefore, the eigenvalues are symmetric with respect to $t \to -t$.

The Hubbard model also has partial particle-hole symmetry. Let

$$d^\dagger_{i\uparrow} = c_{i\uparrow}(-1)^{\varepsilon(i)}, \quad d_{i\uparrow} = c^\dagger_{i\uparrow}(-1)^{\varepsilon}(i)$$

$$d^\dagger_{i\downarrow} = c^\dagger_{i\downarrow}, \quad d_{i\downarrow} = c_{i\downarrow}$$

Then,

$$c^\dagger_{i\uparrow} c_{j\uparrow} = d_{i\uparrow} d^\dagger_{j\uparrow} (-1)^{\varepsilon(i)+\varepsilon(j)} = -d_{i\uparrow} d^\dagger_{j\uparrow} = d^\dagger_{j\uparrow} d_{i\uparrow}$$

So,

$$c^\dagger_{i\uparrow} c_{j\uparrow} + c^\dagger_{j\uparrow} c_{i\uparrow} = d^\dagger_{i\uparrow} d_{j\uparrow} + d^\dagger_{j\uparrow} d_{i\uparrow}$$

and

$$n_{i\uparrow} \to d_{i\uparrow} d^\dagger_{i\uparrow} = -d^\dagger_{i\uparrow} d_{i\uparrow} + 1 \implies N_\uparrow = V - N_\uparrow$$

So,

$$\begin{aligned} \hat{H} &\to -t \sum_{\langle ij\rangle\sigma} (d^\dagger_{i\sigma} d_{j\sigma} + d^\dagger_{j\sigma} d_{i\sigma}) - U \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} + U \sum_i d^\dagger_{i\downarrow} d_{i\downarrow} \\ &\implies E(U, N_\uparrow, \downarrow) = E(-U, V - N_\uparrow, N_\downarrow) + U N_\downarrow \end{aligned}$$

If $N_\uparrow = N_\downarrow = \frac{V}{2}$ (half-filling case), then

$$\boxed{E(U, V/2, V/2) = E(-U, V/2, V/2) + \frac{UV}{2}}$$

Therefore, up to a constant, energies are symmetric for $U \to -U$ at half-filling. Let's look at spin next.

$$\left[\hat{H}, \sum_k n_{k\sigma'}\right] = -t \sum_{\langle ij\rangle\sigma} [c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}, n_{k\sigma'}]$$

and since $[n_{k\sigma}, n_{k'\sigma'}] = 0$

$$\begin{aligned} &= -t \sum_{\langle ij\rangle} \sum_k \left(\delta_{ik}(-c^\dagger_{i\sigma'} c_{j\sigma'} + c^\dagger_{j\sigma'} c_{i\sigma'}) + \delta_{jk}(c^\dagger_{i\sigma'} c_{j\sigma'} - c^\dagger_{j\sigma'} c_{i\sigma}) \right) \\ &= -t \sum_{\langle ij\rangle} (-c^\dagger_{i\sigma'} c_{j\sigma'} + c^\dagger_{j\sigma'} c_{i\sigma'} + c^\dagger_{i\sigma'} c_{j\sigma'} - c^\dagger_{j\sigma'} c_{i\sigma'}) \\ &= 0. \end{aligned}$$

So $\hat{S}_z = \frac{1}{2}\sum_i (n_{i\uparrow} - n_{i\downarrow})$ and $\hat{N} = \sum_i (n_{i\uparrow} + n_{i\downarrow})$ both commute with $\hat{H}$. Hence, we can have simultaneous eigenstates with definite S_z and N.

$$\left[H, \sum_k c^\dagger_{k\uparrow} c_{k\downarrow}\right] = -t \sum_{<ij>\sigma} \sum_k [c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}, c^\dagger_{k\uparrow} c_{k\downarrow}] + U \sum_i \sum_k [n_{i\uparrow} n_{i\downarrow}, c^\dagger_{k\uparrow} c_{k\downarrow}]$$

but $[c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma},c^\dagger_{k\uparrow}c_{k\downarrow}]=\delta_{ik}(c^\dagger_{j\uparrow}c_{i\downarrow}-c^\dagger_{i\uparrow}c_{j\downarrow})\ +\delta_{jk}(c^\dagger_{i\uparrow}c_{j\downarrow}-c^\dagger_{j\uparrow}c_{i\downarrow})$. When summed over $\langle ij\rangle$, this vanishes. Then,

$$\begin{aligned}[n_{i\uparrow}n_{i\downarrow},c^\dagger_{k\uparrow}c_{k\downarrow}]&=n_{i\uparrow}[n_{i\downarrow},c^\dagger_{k\uparrow}c_{k\downarrow}]+[n_{i\uparrow},c^\dagger_{k\uparrow}c_{k\downarrow}]n_{i\downarrow}\\&=-n_{i\uparrow}c^\dagger_{i\uparrow}c_{i\downarrow}\delta_{ik}+c^\dagger_{i\uparrow}c_{i\downarrow}\delta_{ik}\\&=0.\end{aligned}$$

This means that $[\hat{H},\hat{S}^+]=[\hat{H},\hat{S}^-]=0$ so S^2 and S_z are good quantum numbers.

Now, look at pseudospin. We already showed that $[\hat{H},\hat{J}_z]=0$ where $\hat{J}_z=\frac{1}{2}(\hat{N}-V)$. Define:

$$\begin{aligned}\hat{J}^+&=\sum_i c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)}\text{ (pair creation operator)}\\\hat{J}^-&=\sum_i c_{i\downarrow}c_{i\uparrow}(-1)^{\varepsilon(i)}\text{ (pair destruction operator)}\end{aligned}$$

$$\begin{aligned}[\hat{T},\hat{J}^+]=&-t\sum_{\langle ij\rangle\sigma}\sum_k[c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma},c^\dagger_{k\sigma}c^\dagger_{k\downarrow}(-1)^{\varepsilon(k)}]\\=&-t\sum_{<ij>}\sum_k\Big(\delta_{ik}(c^\dagger_{j\uparrow}c^\dagger_{k\downarrow}(-1)^{\varepsilon(k)}-c^\dagger_{j\downarrow}c^\dagger_{k\uparrow}(-1)^{\varepsilon(k)})+\delta_{jk}(c^\dagger_{i\uparrow}c_{k\downarrow}(-1)^{\varepsilon(k)}-c^\dagger_{i\downarrow}c^\dagger_{k\uparrow}(-1)^{\varepsilon(k)})\Big)\\=&-t\sum_{\langle ij\rangle}(c^\dagger_{j\uparrow}c^\dagger_{i\downarrow}-c^\dagger_{j\downarrow}c^\dagger_{i\uparrow})(-1)^{\varepsilon(i)}+(c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}-c^\dagger_{i\downarrow}c^\dagger_{j\uparrow})(-1)^{\varepsilon(j)}\\=&\,0\end{aligned}$$

and

$$\begin{aligned}[\hat{U},\hat{J}^+]&=U\sum_{ij}[n_{i\uparrow}n_{i\downarrow},c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}(-1)^{\varepsilon(j)}]\\&=U\sum_{ij}\delta_{ij}\left(c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}n_{i\downarrow}(-1)^{\varepsilon(i)}+n_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)}\right)\\&=U\sum_i(c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}c^\dagger_{i\downarrow}c_{i\downarrow}(-1)^{\varepsilon(i)}+c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)})\\&=UJ^+.\end{aligned}$$

So $[\hat{H},\hat{J}^+]=U\hat{J}^+$. Therefore, $\hat{J}^+$ is a raising operator for $\hat{H}$ and j,m_j are good quantum numbers. One can also show that

$$\begin{aligned}[J^z,J^\pm]&=\pm J^\pm\\[J^+,J^-]&=2J^z,\end{aligned}$$

which means that $\hat{J}$ acts like an angular momentum operator just like $\hat{S}$ does. Also,

$$E(m_j)=E(-j)+(m_j+J)U$$

You will examine this on the homework and also see in the next lecture. m_j governs the number of particles as m_j increases by 1, the number of particles increases by 2 as we have added a pair with J^+.

4 Limiting cases

When $U = 0$, use the momentum space representation and bath tub principle to fill in the noninteracting levels (always a metal).

When $U \to \infty$, use the real space representation. There is no double occupancy and at half-filling there is one electron per site which are frozen and cannot move (insulator). So we will have a metal-insulator phase transition as a function of U.

For $d = 1$, $U_{mit} = 0^+$ and for $d \to \infty$, $U_{mit} \approx$ bandwidth.