Hubbard model

Original Mott picture

Consider a collection of H atoms.

As we bring the atoms closer 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.

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

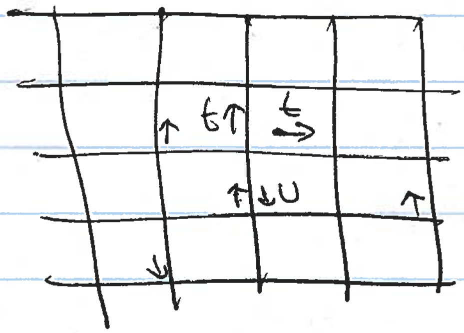
$\langle ij \rangle$ counts nearest neighbor pairs once

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

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



Let's examine $\hat{H}$ in momentum space (Bloch or plane-wave basis)

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

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

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

substitute into $\hat{H}$

$$\hat{H} = -t \sum_{\langle ij\rangle\sigma} \frac{1}{V} \sum_{kk'} \left(e^{-ik\cdot r_i + ik'\cdot r_j} a^\dagger_{k\sigma} a_{k'\sigma} + e^{ik\cdot r_i - ik'\cdot r_j} a^\dagger_{k'\sigma} a_{k\sigma} \right)$$

$$+ U \sum_i \frac{1}{V^2} \sum_{k_1k_2k_3k_4} e^{-i(k_1-k_2)\cdot r_i - i(k_3-k_4)\cdot r_i} a^\dagger_{k_1\uparrow} a_{k_2\uparrow} a^\dagger_{k_3\downarrow} a_{k_4\downarrow}$$

note that for nearest-neighbor pairs $r_j = r_i + \delta$ with δ = 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

$$\sum_{k\sigma} \varepsilon_k a^\dagger_{k\sigma} a_{k\sigma} \text{ with } \varepsilon_k = -t \frac{1}{2} \sum_\delta \left(e^{ik\cdot\delta} + e^{-ik\cdot\delta} \right)$$

$$= -t \sum_\delta \cos(k\cdot\delta)$$

and the second term becomes

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

so we find

$$\hat{H}_{\text{Hubbard}} \underset{\substack{\text{momentum}\\ \text{space}}}{=} \sum_{k\sigma}\varepsilon_k a^{+}_{k\sigma}a_{k\sigma} + \frac{U}{V}\sum_{kk'q} a^{+}_{k+q\uparrow}a_{k\uparrow}a^{+}_{k'-q\downarrow}a_{k'\downarrow}$$

Note that in real space the first term (KE) is complicated, but the second (PE) 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

Symmetries of the Hubbard model:

suppose the lattice is bipartite $\Rightarrow$ $t_{ij} \neq 0$ only if $i \in A$ and $j \in B$ or $i \in B$ and $j \in A$ never AA or BB

examples with nearest-neighbor hopping:

Simple cubic lattice

Square lattice

body centered cubic lattice

Not face centered cubic lattice

not triangular lattice

Then $t \leftrightarrow -t$ is a symmetry.

proof: define $c'^{+}_{i\sigma} = (-1)^{\varepsilon(i)} c^{+}_{i\sigma}$ $\quad c'_{i\sigma} = (-1)^{\varepsilon(i)} c_{i\sigma}$

$$\varepsilon(i) = 1 \quad i \in A, \quad 0 \quad i \in B$$

Then

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

since $c^{+}_{i\sigma} c_{j\sigma} = - c^{+\prime}_{i\sigma} c'_{j\sigma}$ when i, j on different sublattices

$\Rightarrow$ $\boxed{\text{eigenvalues symmetric with respect to } t \to -t}$

Partial particle-hole symmetry

Let $d^{+}_{i\uparrow} = c_{i\uparrow} (-1)^{\varepsilon(i)}$ $\quad d_{i\uparrow} = c^{+}_{i\uparrow} (-1)^{\varepsilon(i)}$

$d^{+}_{i\downarrow} = c^{+}_{i\downarrow}$ $\quad d_{i\downarrow} = c_{i\downarrow}$

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

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

and $n_{i\uparrow} \to d_{i\uparrow} d^{+}_{i\uparrow} = - d^{+}_{i\uparrow} d_{i\uparrow} + 1 \Rightarrow N_{\uparrow} \to V - N_{\uparrow}$

so $\hat{H} \to -t \sum_{\langle ij \rangle \sigma} \left(d^{+}_{i\sigma} d_{j\sigma} + d^{+}_{j\sigma} d_{i\sigma} \right) - U \sum_i d^{+}_{i\uparrow} d_{i\uparrow} d^{+}_{i\downarrow} d_{i\downarrow}$

$\quad + U \sum_i d^{+}_{i\downarrow} d_{i\downarrow}$

$\Rightarrow E(U, N_{\uparrow}, N_{\downarrow}) = E(-U, V - N_{\uparrow}, N_{\downarrow}) + U N_{\downarrow}$

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

$$\boxed{E\left(U, \tfrac{V}{2}, \tfrac{V}{2}\right) = E\left(-U, \tfrac{V}{2}, \tfrac{V}{2}\right) + U\frac{V}{2}}$$

$\Rightarrow$ up to a constant energies are symmetric for $U \to -U$ at half filling.

Spin

k is a spatial index here not momentum

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

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

$$= -t \sum_{\langle ij\rangle} \sum_k [\delta_{ik}(-c^\dagger_{i\sigma'} c_{j\sigma'} + c^\dagger_{j\sigma'} c_{i\sigma'}) + \delta_{jk}(c^\dagger_{i\sigma'} c_{j\sigma'} - c^\dagger_{j\sigma'} c_{i\sigma'})]$$

$$= -t \sum_{\langle ij\rangle} (\cancel{-c^\dagger_{i\sigma'} c_{j\sigma'}} + \cancel{c^\dagger_{j\sigma'} c_{i\sigma'}} + \cancel{c^\dagger_{i\sigma'} c_{j\sigma'}} - \cancel{c^\dagger_{j\sigma'} c_{i\sigma'}})$$

$$= 0$$

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 $\hat{H}$. $\Rightarrow$ can get simultaneous eigenstates with definite S_z and N.

spin raising & lowering ops

$$[H, \sum_k c^\dagger_{k\uparrow} c_{k\downarrow}] = -t \sum_{\langle ij\rangle\sigma} \sum_k [c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}, c^\dagger_{k\uparrow} c_{k\downarrow}]$$

$$+ U \sum_i \sum_k [n_{i\uparrow} n_{i\downarrow}, c^\dagger_{k\uparrow} c_{k\downarrow}]$$

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 $\langle ij\rangle$ k these vanishes.

$$[n_{i\uparrow} n_{i\downarrow}, c^\dagger_{k\uparrow} c_{k\downarrow}] = n_{i\uparrow} [n_{i\downarrow}, c^\dagger_{k\uparrow} c_{k\downarrow}] + [n_{i\uparrow}, c^\dagger_{k\uparrow} c_{k\downarrow}] n_{i\downarrow}$$

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

$$= 0$$

so $[\hat H, \hat S^+]=0$ similarly $[\hat H, \hat S^-]=0$

so S^2 and S_z are good quantum numbers.
S, m_S

Pseudospin

already showed $[\hat H, \hat J_z]=0$ $\quad \hat J_z = \frac{1}{2}(\hat N - V)$

Define $\hat J^+ = \sum_i c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)}$ pair creation operator

$\hat J^- = \sum_i c_{i\downarrow} c_{i\uparrow}(-1)^{\varepsilon(i)}$ pair destruction operator

$$[\hat T, \hat J^+] = -t\sum_{\langle ij\rangle\sigma}\sum_k \left[c^\dagger_{i\sigma}c_{j\sigma}+c^\dagger_{j\sigma}c_{i\sigma},\ c^\dagger_{k\uparrow}c^\dagger_{k\downarrow}(-1)^{\varepsilon(k)}\right]$$

$$= -t\sum_{\langle ij\rangle}\sum_k \Big[\delta_{ik}\left[c^\dagger_{j\uparrow}c^\dagger_{k\downarrow}(-1)^{\varepsilon(k)} \pm c^\dagger_{j\downarrow}c^\dagger_{k\uparrow}(-1)^{\varepsilon(k)}\right)$$

$$+\,\delta_{jk}\left[c^\dagger_{i\uparrow}c^\dagger_{k\downarrow}(-1)^{\varepsilon(k)} \mp c^\dagger_{i\downarrow}c^\dagger_{k\uparrow}(-1)^{\varepsilon(k)}\right]$$

$$= -t\sum_{\langle ij\rangle}\left(c^\dagger_{j\uparrow}c^\dagger_{i\downarrow} - c^\dagger_{j\downarrow}c^\dagger_{i\uparrow}\right)(-1)^{\varepsilon(i)} + \left(c^\dagger_{i\uparrow}c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow}c^\dagger_{j\uparrow}\right)(-1)^{\varepsilon(j)}$$

$(-1)^{\varepsilon(i)} = -(-1)^{\varepsilon(j)}$

$= 0$

$$[\hat U, \hat J^+] = U\sum_{ij}\left[n_{i\uparrow}n_{i\downarrow},\ c^\dagger_{j\uparrow}c^\dagger_{j\downarrow}(-1)^{\varepsilon(j)}\right]$$

$$= U\sum_{ij}\delta_{ij}\left[c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}n_{i\downarrow}(-1)^{\varepsilon(i)} + n_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)}\right]$$

0

$$= U\sum_i\left[c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\cancel{c^\dagger_{i\downarrow}}c_{i\downarrow}(-1)^{\varepsilon(i)} + c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}(-1)^{\varepsilon(i)}\right]$$

$= U J^+$

so $[\hat{H}, \hat{J}^+] = U \hat{J}^+$

$\Rightarrow$ $\boxed{\hat{J}^+ \text{ is a raising operator for } \hat{H}}$

$\Rightarrow$ j and m_j are good quantum numbers

(one can show $[J^z, J^\pm] = \pm J^\pm$
$[J^+, J^-] = 2J^z$

$\Rightarrow$ $\hat{J}$ acts like an angular momentum operator, just like $\hat{S}$ does.

$\Rightarrow$ $E(m_j) = E(-j) + (m_j + j)U$

You will examine this on the HW and also see in next lecture.

m_j governs the number of particles
as m_j increases by 1, number of particles increases by 2 as we have added a pair with J^+

limits $U \to 0$, $U \to \infty$

$U \to 0$ use momentum space rep & bath tub principle
fill in non interacting levels — always a metal

$U \to \infty$ use real space rep $\Rightarrow$ no double occupancy $\Rightarrow$ at half filling one electron per site - frozen and cannot move
$\Rightarrow$ insulator so metal-insulator transition as a fn of U

for $d=1$ $U_{crit} = 0^+$ (famous Lieb-Wu Bethe ansatz solution)

for $d \to \infty$ $U_{crit} \sim$ bandwidth for $d \geq 2$ expect $U_{crit} \sim$ bandwidth.
but exact solution is still unknown