Phys 726 – Lecture 12

Hubbard model

* prototype model for strong electronic correlations

→ competition between kinetic energy and Coulomb repulsion terms

$$\hat{H} = \hat{H}_t + \hat{H}_u$$

→ kinetic term takes the form of a bilinear hopping process and gives rise to a tight-binding band structure

$$\sum_{ij} t_{ij} (c_i^\dagger c_j + c_j^\dagger c_i) = \sum_{\vec{R}\vec{R}'} t(R-R')(c_R^\dagger c_{R'} + c_{R'}^\dagger c_R)$$

$$= \sum_k \varepsilon_k c_k^\dagger c_k \quad \text{with } \varepsilon_k = \sum_R e^{ik\cdot R} t(R)$$

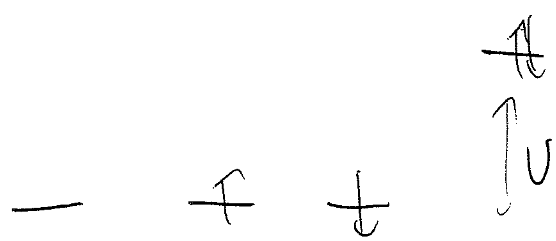
whose lowest-energy state is delocalized

diagonal in the crystal momentum representation

$$c_{k=0}^\dagger = \sum_R c_R^\dagger$$

→ Coulomb term takes the form of an onsite, spin-dependent density-density measurement, which has the effect of penalizing double occupancy

$$\hat{H}_u = U \sum_i \hat{n}_{i\uparrow} n_{i\downarrow} = U \sum_{\vec{R}} \hat{n}_{\vec{R}\uparrow} \hat{n}_{\vec{R}\downarrow}$$



<u>EXAMPLE</u>: Consider the two-site version of this model

$$\hat{H} = -t \sum_{\alpha=\uparrow,\downarrow} \left(c^{\dagger}_{1\alpha} c_{2\alpha} + c^{\dagger}_{2\alpha} c_{1\alpha} \right) + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

① How many basis states are there in the two-electron sector of the Hilbert space?

Six states $|\phi_n\rangle$ of the form $c^\dagger_{i\alpha} c^\dagger_{j\beta} |vac\rangle$

$$|\phi_1\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\downarrow} |vac\rangle = |\uparrow,\downarrow\rangle$$

$$|\phi_2\rangle = c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} |vac\rangle = |\downarrow,\uparrow\rangle$$

$$|\phi_3\rangle = c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} |vac\rangle = |\uparrow,\uparrow\rangle$$

$$|\phi_4\rangle = c^\dagger_{1\downarrow} c^\dagger_{2\downarrow} |vac\rangle = |\downarrow,\downarrow\rangle$$

$$|\phi_5\rangle = c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} |vac\rangle = |\uparrow\downarrow,0\rangle$$

$$|\phi_6\rangle = c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} |vac\rangle = |0,\uparrow\downarrow\rangle$$

↑ defined using the convention that 1 precedes 2 and ↑ precedes ↓ when reading the operator string from left to right.

$\{|\phi_n\rangle\}$ forms an orthonormal set. Check that $\langle\phi_n|\phi_m\rangle = \delta_{n,m}$.

The other combinations vanish as a result of Pauli exclusion

e.g. $c^\dagger_{1\uparrow} c^\dagger_{1\uparrow} |vac\rangle = (c^\dagger_{1\uparrow})^2 |vac\rangle = 0$

(2) What is the matrix form of the Hamiltonian in this basis?

$$H_{m,n} = \langle \phi_m | \hat{H} | \phi_n \rangle$$

$\hat{H}_t$ changes the electronic configuration whereas $\hat{H}_u$ is diagonal in the occupation number representation

$$H_{11} = \langle \phi_1 | \hat{H} | \phi_1 \rangle = \langle \uparrow, \downarrow | \hat{H}_u | \uparrow, \downarrow \rangle = 0$$
$$H_{22} = \langle \phi_2 | \hat{H} | \phi_2 \rangle = \langle \downarrow, \uparrow | \hat{H}_u | \downarrow, \uparrow \rangle = 0$$
$$H_{33} = \langle \phi_3 | \hat{H} | \phi_3 \rangle = \langle \uparrow, \uparrow | \hat{H}_u | \uparrow, \uparrow \rangle = 0$$
$$H_{44} = \langle \phi_4 | \hat{H} | \phi_4 \rangle = \langle \downarrow, \downarrow | \hat{H}_u | \downarrow, \downarrow \rangle = 0$$
$$H_{55} = \langle \phi_5 | \hat{H} | \phi_5 \rangle = \langle \uparrow\downarrow, 0 | \hat{H}_u | \uparrow\downarrow, 0 \rangle = U$$
$$H_{66} = \langle \phi_6 | \hat{H} | \phi_6 \rangle = \langle 0, \uparrow\downarrow | \hat{H}_u | 0, \uparrow\downarrow \rangle = U$$

Hilbert space breaks into a low- and a high-energy sector

Think about what the hopping does in this case.

$$|\uparrow,\downarrow\rangle \xrightarrow{H_t} |\uparrow\downarrow,0\rangle\ ,\ |0,\uparrow\downarrow\rangle$$

$$|\downarrow,\uparrow\rangle \longrightarrow |\uparrow\downarrow,0\rangle\ ,\ |0,\uparrow\downarrow\rangle$$

$$|\uparrow,\uparrow\rangle \longrightarrow \phi$$

$$|\downarrow,\downarrow\rangle \longrightarrow \phi$$

$$|\uparrow\downarrow,0\rangle \longrightarrow |\uparrow,\downarrow\rangle\ ,\ |\downarrow,\uparrow\rangle$$

$$|0,\uparrow\downarrow\rangle \longrightarrow |\uparrow,\downarrow\rangle\ ,\ |\downarrow,\uparrow\rangle$$

The offdiagonal terms only connect $|\phi_1\rangle, |\phi_2\rangle$ to $|\phi_5\rangle, |\phi_6\rangle$. So the matrix has the form

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 & ? & ? \\ 0 & 0 & 0 & 0 & ? & ? \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ ? & ? & 0 & 0 & U & 0 \\ ? & ? & 0 & 0 & 0 & U \end{pmatrix}$$

We have to be careful about signs, because of the electrons' exchange property

e.g. $\hat{H}_t |\phi_1\rangle = \hat{H}_t \underbrace{c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |vac\rangle}_{\text{our convention for } |\phi_1\rangle}$

$$= \sum_\alpha (c_{1\alpha}^\dagger c_{2\alpha} + c_{2\alpha}^\dagger c_{1\alpha}) c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |vac\rangle$$

$$= \sum_\alpha (c_{1\alpha}^\dagger c_{2\alpha} c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{2\alpha}^\dagger c_{1\alpha} c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger) |vac\rangle$$

$$= \sum_\alpha \Big(- c_{1\alpha}^\dagger c_{1\uparrow}^\dagger (\delta_{\alpha\downarrow} - \cancelto{0}{c_{2\downarrow}^\dagger c_{2\alpha}})$$

$$+ c_{2\alpha}^\dagger c_{2\downarrow}^\dagger (\delta_{\alpha\uparrow} - \cancelto{0}{c_{1\uparrow}^\dagger c_{1\alpha}}) \Big) |vac\rangle$$

$$= - c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger |vac\rangle + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |vac\rangle$$

$$= + c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |vac\rangle + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |vac\rangle$$

$$= |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle$$

$$\hat{H}_t |\phi_2\rangle = \hat{H}_t \underbrace{c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} |vac\rangle}_{|\phi_2\rangle = |\downarrow,\uparrow\rangle}$$

$$= \sum_\alpha \left(c^\dagger_{1\alpha} c_{2\alpha} + c^\dagger_{2\alpha} c_{1\alpha} \right) c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} |vac\rangle$$

$$= \sum_\alpha \left(c^\dagger_{1\alpha} \underset{\uparrow\, \delta_{\alpha,\uparrow}}{c_{2\alpha}} c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} + c^\dagger_{2\alpha} \underset{\uparrow\, \delta_{\alpha,\downarrow}}{c_{1\alpha}} c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} \right) |vac\rangle$$

$$= \left(c^\dagger_{1\uparrow} c_{2\uparrow} c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} + c^\dagger_{2\downarrow} c_{1\downarrow} c^\dagger_{1\downarrow} c^\dagger_{2\uparrow} \right) |vac\rangle$$

$$= \Big(- c^\dagger_{1\uparrow} c^\dagger_{1\downarrow} \big(1 - \cancelto{0}{c^\dagger_{2\uparrow} c_{2\uparrow}}\big)$$

$$- c^\dagger_{2\uparrow} c^\dagger_{2\downarrow} \big(1 - c^\dagger_{1\uparrow} c_{1\uparrow}\big) \Big) |vac\rangle$$

$$= - |\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle$$

$$H = \begin{pmatrix} U & 0 & 0 & 0 & t & t \\ 0 & 0 & 0 & 0 & -t & -t \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ t & -t & 0 & 0 & U & 0 \\ t & -t & 0 & 0 & 0 & U \end{pmatrix}$$

Diagonalizing gives

$$|\psi_1\rangle = |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle \qquad E_1 = U$$

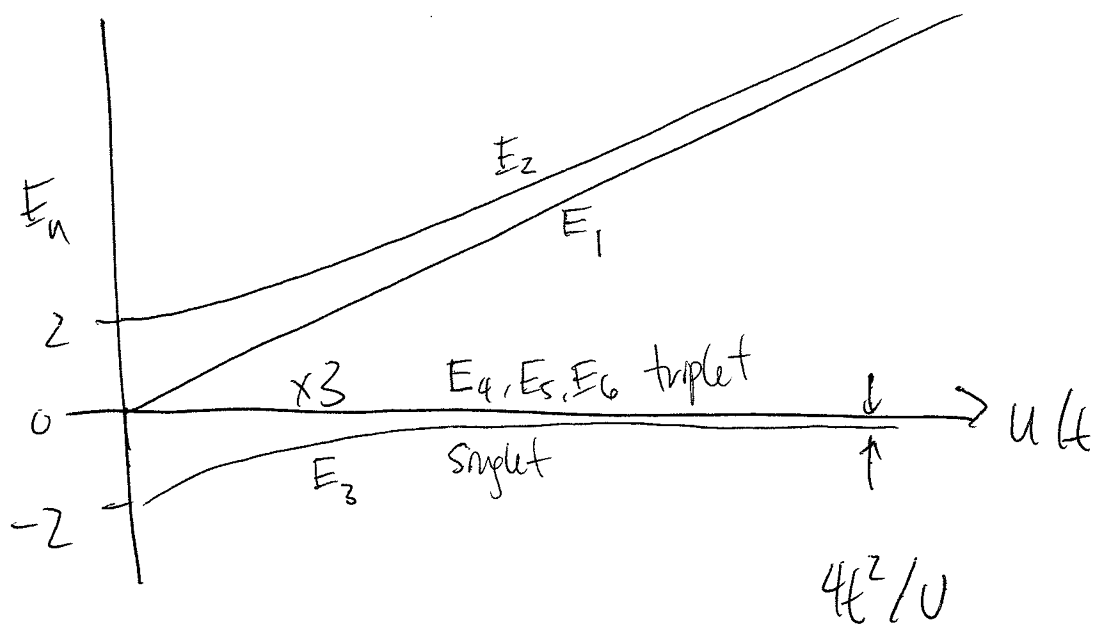
$$|\psi_{2,3}\rangle = 2t\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + e^{\pm}\left(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle\right)$$

$$E_{2,3} = e^{\pm} = \frac{1}{2}\left(U \pm \sqrt{U^2 + 16t^2}\right)$$

$$|\psi_4\rangle = |\uparrow,\uparrow\rangle \qquad E_4 = 0$$

$$|\psi_5\rangle = |\downarrow,\downarrow\rangle \qquad E_5 = 0$$

$$|\psi_6\rangle = |\uparrow\downarrow\rangle + |\downarrow,\uparrow\rangle \qquad E_6 = 0$$



$$E_{2,3} = \frac{1}{2}\left(U \pm \sqrt{U^2+16t^2} \right)$$

$$= \frac{1}{2}\left(U \pm U\sqrt{1+\frac{16t^2}{U^2}} \right)$$

$$= \frac{1}{2}\left(U \pm U\left[1+\frac{8t^2}{U^2}+\cdots\right] \right)$$

$$= \begin{cases} U \\ -\frac{4t^2}{U} \end{cases} \quad \text{as } U\to\infty$$

$$\hat{H}_{eff} = J\vec{S}_1\cdot\vec{S}_2 = -\frac{4t^2}{U}\, \frac{1}{2}c^\dagger_{1\alpha}\vec{\sigma}_{\alpha\beta}c_{1\beta}\cdot\frac{1}{2}c^\dagger_{2\mu}\vec{\sigma}_{\mu\nu}c_{2\nu}$$