Hubbard model. (J. Hubbard 1963).

(~~b.~~ "extension" Heitler-London 1927).
H_2

tight binding model (LCAO) does not include interactions

simplest model taking interactions into account (one band one orbital per site)

$$H = -t \underbrace{\sum_{ij,\sigma} c^{\dagger}_{j\sigma} c_{i\sigma}}_{\text{hopping}} + U \underbrace{\sum_i n_{i\uparrow} n_{i\downarrow}}_{\text{interaction}}$$

nearest neighbor: i & j adjacent

interaction term: $n_{i\uparrow} n_{i\downarrow} = c^{\dagger}_{i\uparrow} c_{i\uparrow} c^{\dagger}_{i\downarrow} c_{i\downarrow}$ $\Rightarrow$ "problem" term

in 1D exact solution Lieb & Wu 1968.

Some remarks / reminders

(1) fermionic operators: $c^{\dagger}_{2\uparrow} |0\rangle = |\cdot, \uparrow, \cdot, \cdot \dots\rangle$

$$c_{3\downarrow} c^{\dagger}_{5\uparrow} |\cdot, \cdot, \downarrow, \cdot, \cdot, \cdot\rangle = |\cdot \cdot \cdot \cdot \uparrow \cdot \cdot\rangle$$

$$c_{2\uparrow} |0\rangle = 0.$$

etc.

operators anticommute.

$$\{c_{i\sigma}, c^{\dagger}_{j\sigma'}\} = c_{i\sigma} c^{\dagger}_{j\sigma'} + c^{\dagger}_{j\sigma'} c_{i\sigma} = \delta_{ij} \delta_{\sigma\sigma'}$$

$$\{c_{i\sigma}, c_{j\sigma'}\} = \{c^{\dagger}_{i\sigma}, c^{\dagger}_{j\sigma'}\} = 0.$$

2 partition function $Z \equiv Tr\left[e^{-\beta(\tilde{H}-\mu\tilde{n})} \right]$

$\beta = 1/kT$; μ : chem. pot.

expect. value operator A : $\langle A \rangle = \frac{1}{Z} Tr\left[A\, e^{-\beta(\tilde{H}-\mu\tilde{n})} \right]$

example single state with 0 or 1 electrons, energy ε

$$H = \varepsilon c^{+} c \quad (= \varepsilon \tilde{n}) \qquad c^{+}c|0\rangle = 0, \; c^{+}c|1\rangle = 1.$$

$$Z = \langle 0| e^{-\beta(\tilde{H}-\mu\tilde{n})} |0\rangle + \langle 1| e^{-\beta(\tilde{H}-\mu\tilde{n})} |1\rangle.$$

$$= 1 + e^{-\beta(\varepsilon-\mu)}$$

average occupation

$$\langle n \rangle = \frac{1}{Z} \left\{ \langle 0| \hat{n} e^{-\beta(\hat{H}-\mu\hat{n})} |0\rangle + \langle 1| \tilde{n} e^{-\beta(\tilde{H}-\mu\tilde{n})} |1\rangle \right\}$$

$$= \frac{1}{Z} \left\{ 0 + e^{-\beta(\varepsilon-\mu)} \right\}$$

$$= \frac{e^{-\beta(\varepsilon-\mu)}}{1 + e^{-\beta(\varepsilon-\mu)}}$$

F.D. distribution.

Back to hubbard model.

two extremes: (A) $U \neq 0$ $t=0$ & (B) $U=0$ $t \neq 0$.

(A) $t=0$. no hopping $\Rightarrow$ all sites independent.

$H = U n_\uparrow n_\downarrow$

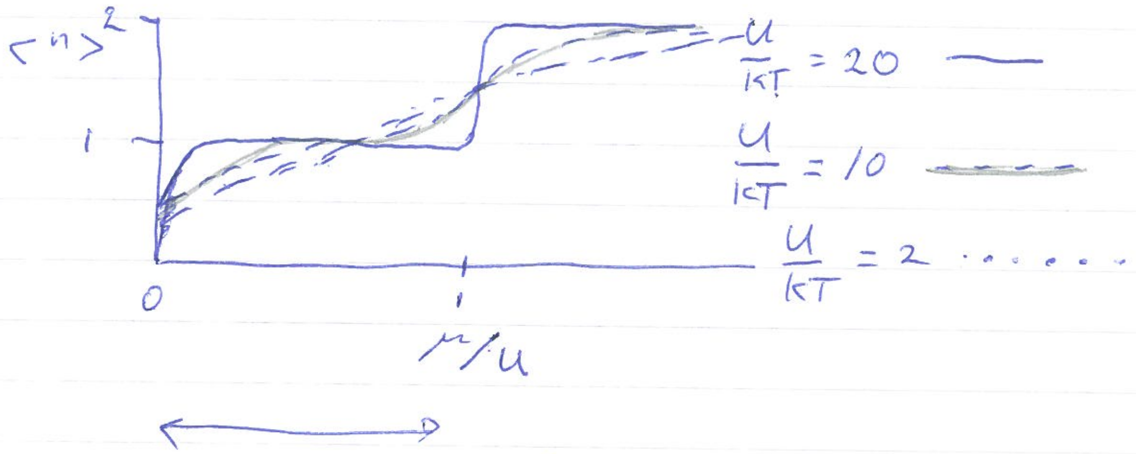
possible states of a single site: $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$.

what is the occupation? $\rightsquigarrow \; = \tilde{n}_\downarrow + \tilde{n}_\uparrow$

$$Z = \sum_s \langle s| e^{-\beta(\tilde{H} - \mu\tilde{n})} |s\rangle = 1 + e^{\beta\mu} + e^{\beta\mu} + e^{-\beta U + 2\beta\mu}$$

$$\left[e^{-\beta(\hat{H}-\mu\tilde{n})}|0\rangle = e^{0} \;;\; e^{-\beta(\hat{H}-\mu n)} \cancel{|\uparrow\rangle} = e^{\beta\mu}, \text{ etc.} \right]$$

then
$$\langle n\rangle = \frac{1}{Z}\sum_s \langle s| \tilde{n}_\downarrow + \tilde{n}_\uparrow |s\rangle = \frac{2\left(e^{\beta\mu} + e^{-\beta U + 2\beta\mu}\right)}{1 + 2e^{\beta\mu} + e^{-\beta U + 2\beta\mu}}$$



adding addl. particle costs U.

$\Rightarrow$ Hubbard gap.

(B) other limit: $U = 0$ (tight binding).

easiest in reciprocal space

$$c^{+}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_{l} e^{ikl} c^{+}_{l\sigma} \qquad k = \frac{2\pi n}{N} \quad \text{(periodic boundary cond.)}$$

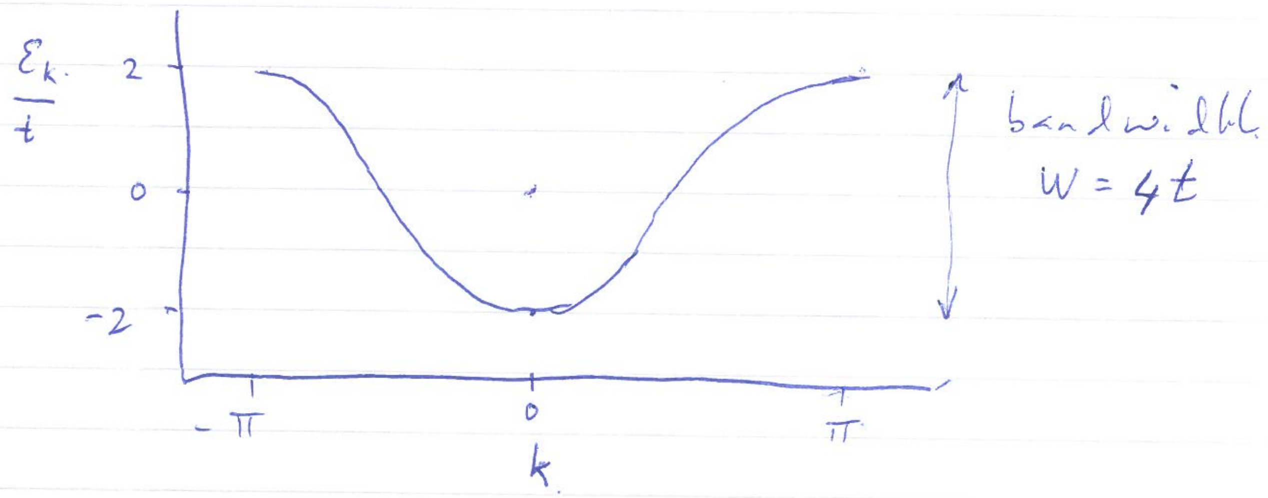
then $H = -t \sum_{\langle jl \rangle \sigma} c^{+}_{j\sigma} c_{l\sigma} = -\frac{t}{N} \sum_{k,k'} \sum_{\langle jl \rangle \sigma} e^{ikj} e^{-ik'l} c^{+}_{k\sigma} c_{k'\sigma}$

$$= -\frac{t}{N} \sum_{kk'\sigma} c^{+}_{k\sigma} c_{k'\sigma} \sum_{j} \left\{ e^{ikj} e^{-ik'(j+1)} + e^{ikj} e^{-ik'(j-1)} \right\} =$$

$$= -t \sum_{kk'\sigma} c^{+}_{k\sigma} c_{k'\sigma} \underbrace{\left[e^{-ik'} + e^{ik'} \right]}_{2\cos k'} \underbrace{\frac{1}{N} \sum_{j} e^{i(k-k')j}}_{\delta_{kk'}}$$

$$= -t \sum_{k\sigma} c^{+}_{k\sigma} c_{k\sigma} \, 2\cos(k') = \sum_{k\sigma} \varepsilon_k c^{+}_{k\sigma} c_{k\sigma}$$

$$\varepsilon_k = -2t \cos k$$



H_2 toy model. $\quad H = -t \sum_{\langle ij \rangle \sigma} c_{j\sigma}^{+} c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$

states $\{ |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow\downarrow,-\rangle, |-,\uparrow\downarrow\rangle \}$.

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

+t due to anticomm.

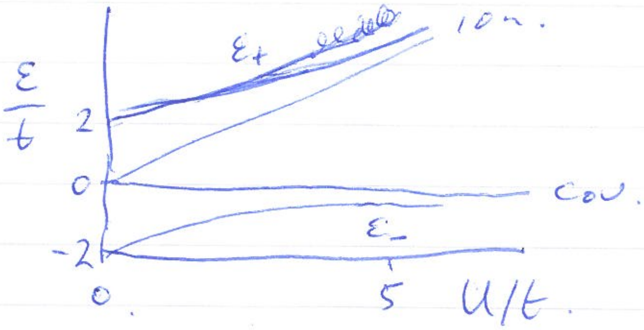
$c_i^{+} c_j + c_j c_i^{+} = 0$ for $i \neq j$

swap $\rightarrow$ (−1)

diagonalize: $\varepsilon_{\pm} = \frac{U}{2} \pm \sqrt{\frac{U^2 + 16t^2}{4}}$

$\varepsilon_{cov} = 0$

$\varepsilon_{ion} = U$



$$\psi_{\pm} = \frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle - \frac{\varepsilon_{\pm}}{2t}\left(|\uparrow\downarrow,-\rangle + |-,\uparrow\downarrow\rangle\right)}{\sqrt{2 + \varepsilon_{\pm}^2/(2t^2)}}$$

$\psi_{cov} = \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right)$

$\psi_{ion} = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow,-\rangle - |-,\uparrow\downarrow\rangle\right)$

Large U: $\varepsilon_{cov} \simeq 0$; $\varepsilon_{ion} = U$.

$\varepsilon_- \simeq -\frac{4t^2}{U} \rightarrow$ AF Ground state.

Mott hubbard transition

insul. $U >> t$: localized $\bar{e}$ (solve in real space).

metal. $U << t$: itinerant $\bar{e}$ (solve in k-space).

at some intermediate U/t : transition metal $\leftrightarrow$ insul.
$\hat{=}$ Mott - transition

half fill, Large U : Antiferromagnetism.

U Large $\rightarrow$ localized states.
kin E term $\rightarrow$ treat in second order. (first order would mix in doubly occ. states).

$$E^{(2)} = \sum_{k \neq n} \frac{|\langle k|V|n\rangle\langle n|V|k\rangle|}{E_n^{(0)} - E_k^{(0)}}$$

$$V = -t \sum_{ij\sigma} c^{+}_{j\sigma} c_{i\sigma} \qquad \uparrow \underset{}{\overset{-\alpha t}{\rightleftarrows}} \downarrow$$

and other way around $\Rightarrow$ factor 2
$\hookrightarrow$ 4 terms in V.
$c^{+}_{2R} c_{2R} c^{+}_{1R} c_{1L}$ etc.

$$E = \frac{-4t^2}{U} \qquad \text{energy gain if AF order.}$$

$\Rightarrow$ effective hamiltonian

$$H = \sum_{ij} J\, \vec{S}_i \vec{S}_j$$

$$J = \frac{4t^2}{U}$$

when not half filled $\Rightarrow$ t-J model.