Lecture 3a

$$\hat{C}_i^\dagger |Vac\rangle = |i\rangle$$

$$\langle r|i\rangle = \psi(r-R_i)$$

$$\hat{C}_j^\dagger \hat{C}_i^\dagger |Vac\rangle = |i,j\rangle$$

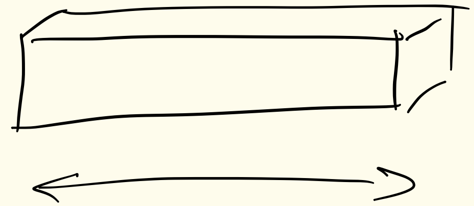
$$\langle r|i,j\rangle = \sqrt{\frac{1}{2}} \begin{vmatrix} \psi_1(r-R_i) & \psi_1(r-R_j) \\ \psi_2(r-R_i) & \psi_2(r-R_j) \end{vmatrix}$$

$$\{C_i^\dagger, C_j^\dagger\} = 0$$

Born-Oppenheimer

Li

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \cancel{\sum_{i,j} U(i,j)}$$



L

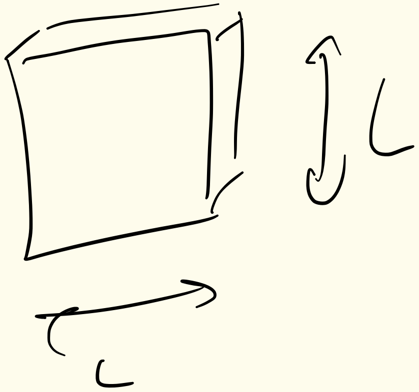
"nearly free electrons"

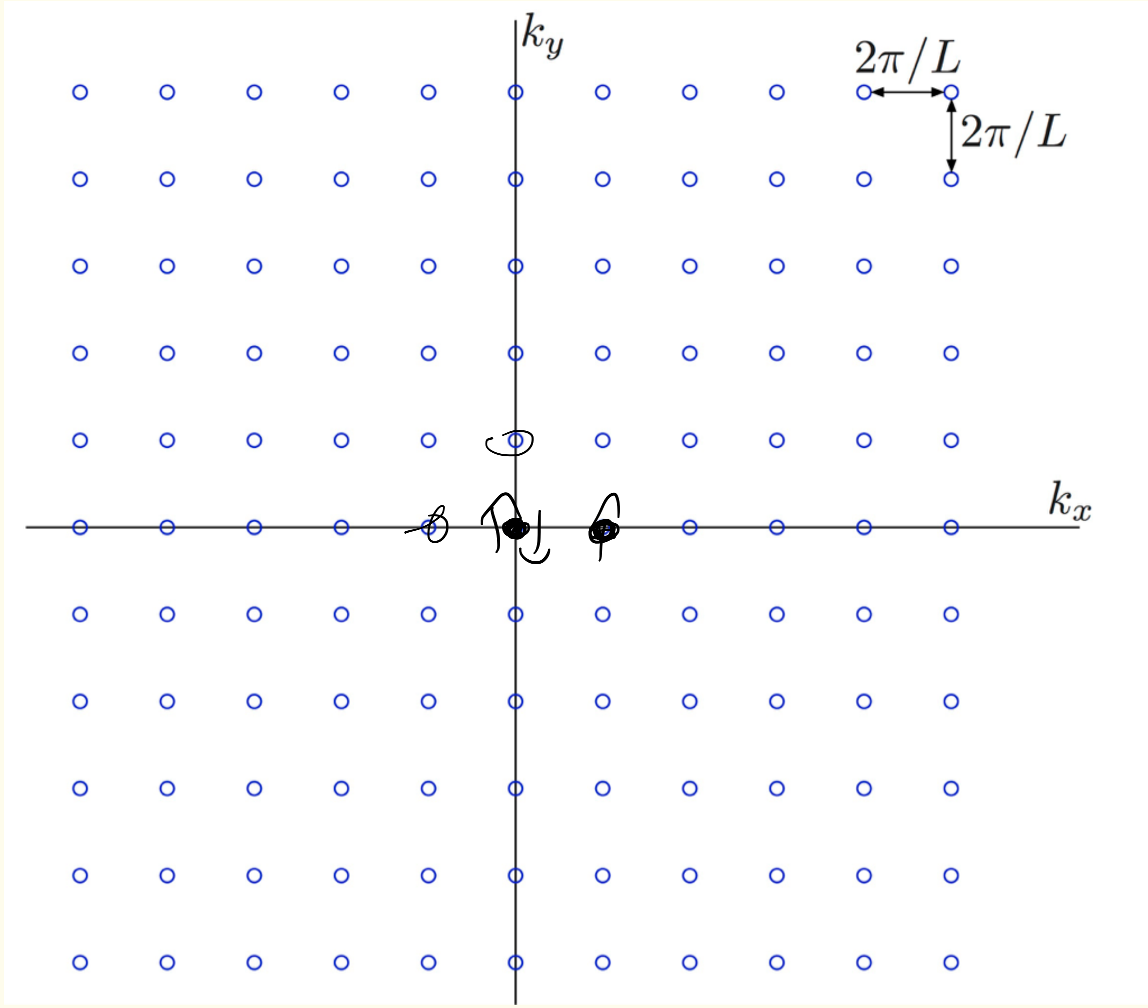
$$k = \frac{2\pi}{L} \cdot n$$

$$\hat{H} = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma}$$

$$n \in \mathbb{Z}$$

2D)



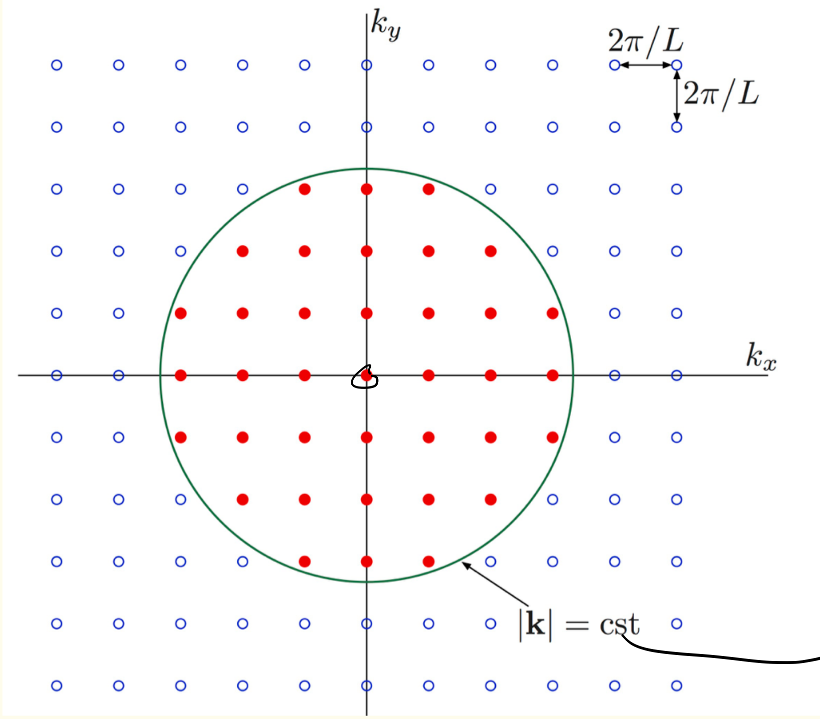


$$k_x = \frac{2\pi}{L} n$$

$$k_y = \frac{2\pi}{L} m$$

$$n, m \in \mathbb{Z}$$

$$\hat{H} = \sum_{k\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^\dagger_{k\sigma} \hat{c}_{k,\sigma}$$

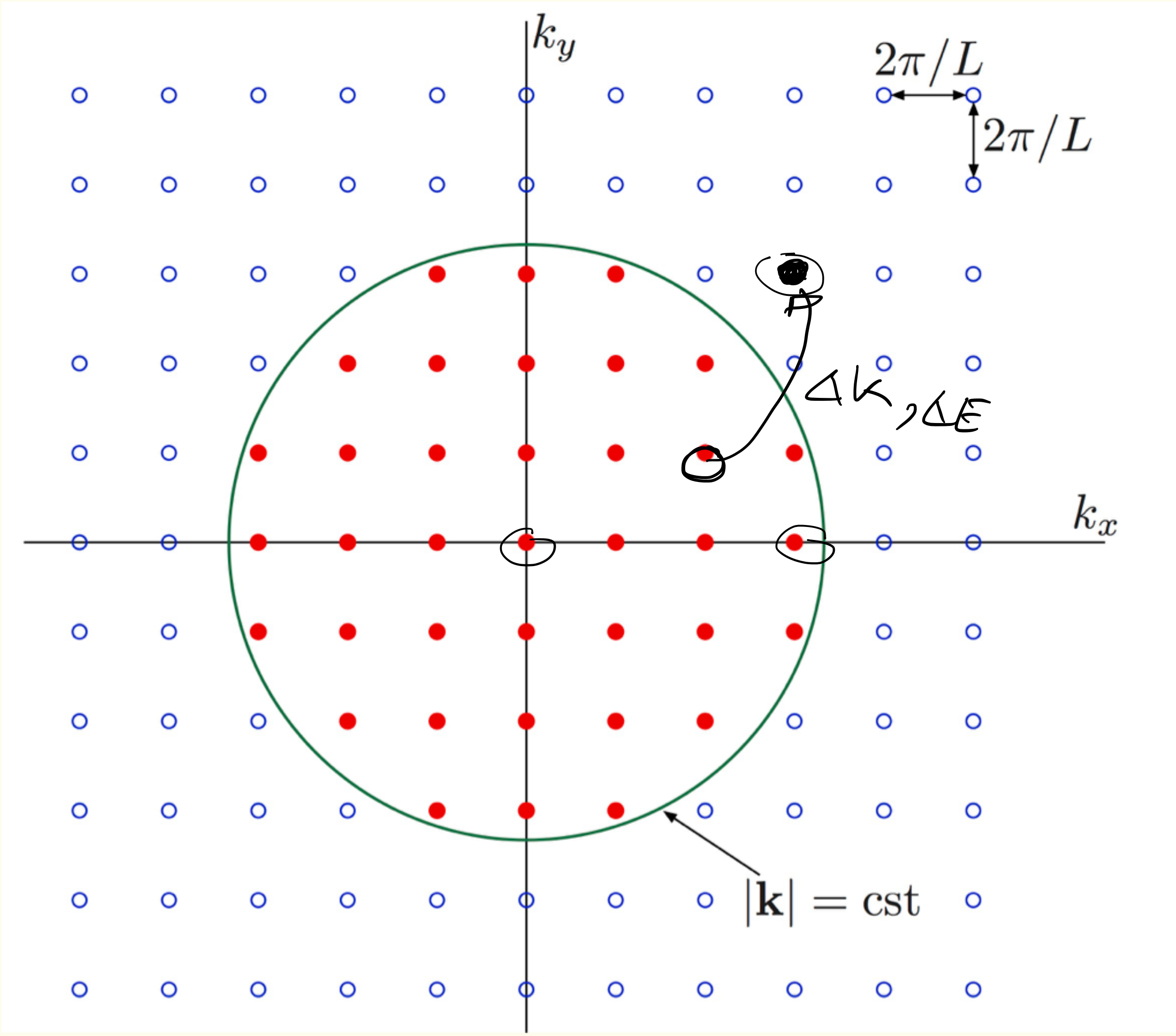


$\equiv k_F$

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

Many-particle ground state

$$|gs\rangle = \prod_{\substack{k,\sigma \\ |k| < k_F}} \hat{c}^\dagger_{k,\sigma} |vac\rangle$$



quasi-particle

m
q
σ
k
E

$$H = H_0 + \sum_{\substack{k,k',q \\ \sigma,\sigma'}} V(q)\, \hat{C}^{\dagger}_{k+q,\sigma} \hat{C}^{\dagger}_{k'+q,\sigma'} \hat{C}_{k',\sigma'} \hat{C}_{k,\sigma}$$

$$V(q) \sim \frac{1}{q^2}$$

"Landau Liquid"

Bohr

$a^d \to$ 1D: a

$K \sim \frac{1}{m a^2}$

$V \sim \frac{e^2}{a}$

atom radius $\to$ $a \ll \frac{1}{e^2 m}$ Bohr radius

$\Leftrightarrow K \gg V$

3D) E_F $\Delta k = \frac{2\pi}{L}$ $Vol = \left(\frac{2\pi}{L}\right)^3$

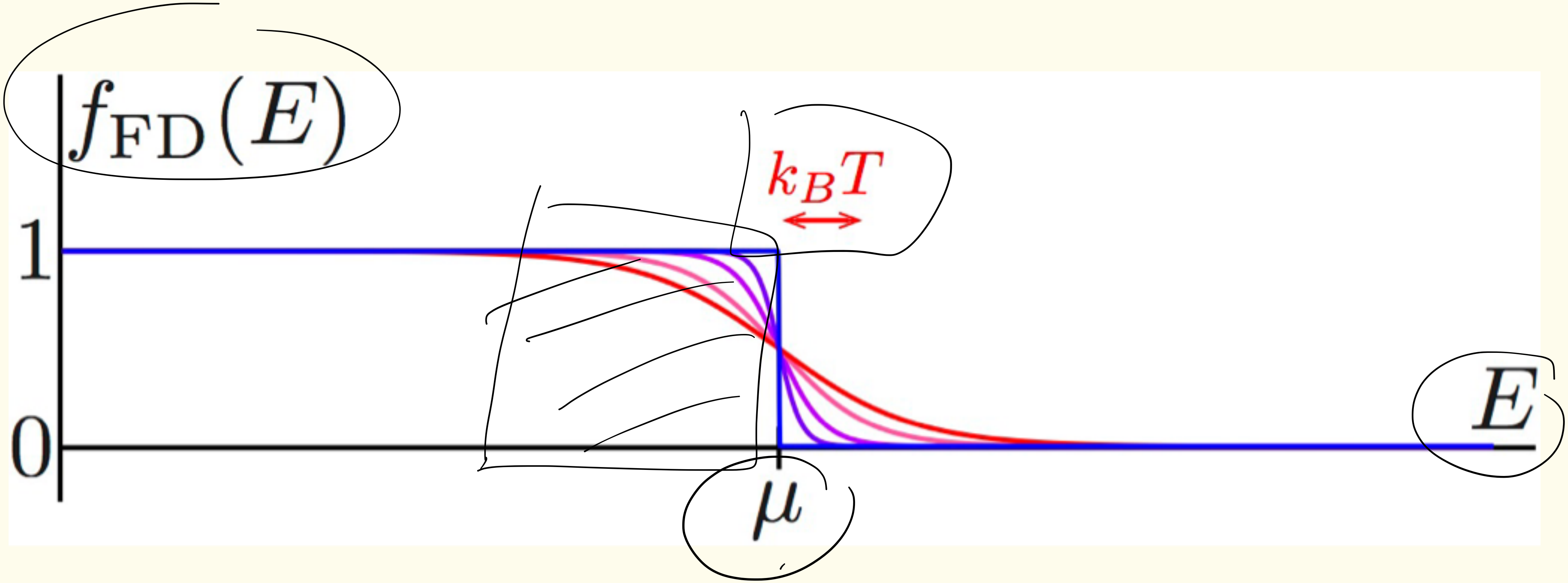
$$\left.\begin{matrix} 2 \\ n \end{matrix}\right\} \quad \#_k = \frac{nN}{2}$$

$$\frac{nN}{2}\left(\frac{2\pi}{L}\right)^3 = \frac{4}{3}\pi k_F^3$$

$$\Rightarrow k_F = \left(\frac{3\pi^2 \rho}{m}\right)^{1/3}$$

$\rho = \frac{m}{V}$

$= \frac{N m_e}{V}$


$f_{\mathrm{FD}}(E)$
1
0
$k_B T$
μ
E

Lecture 3b

D.O.S.

\# between E and $E+dE$: $g(E)\,dE$

\# states ~~k points~~ k, $k+dk$:

$$2\,\frac{4\pi k^2\,dk}{(2\pi/L)^3} = g(E)\,dE \qquad (3D)$$

$$\Longrightarrow \quad g(E) = \frac{L^3}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\sqrt{E}$$

$$\boxed{g(E_F) = 3N/2E_F}$$

Specific heat

$$C = \frac{\partial U}{\partial T}$$

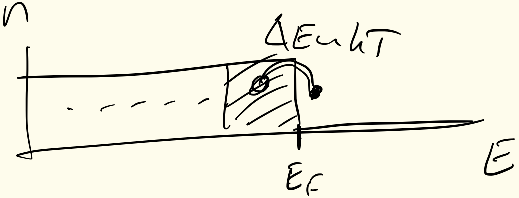
Quantum

$$\# = g(E)\,dE$$

$$\underline{g(E_F)\,kT} = N$$

$$U = g(E_F)\,kT \cdot kT + \text{cst}$$

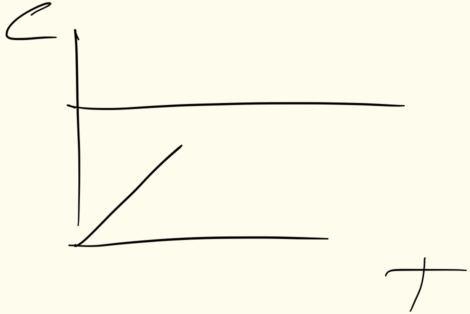
$$\rightarrow C = 3 N k_B \left(T / T_F \right)$$



Classically

$$U = \frac{3}{2} k_B T \cdot N$$

$$\rightarrow C = \frac{3}{2} k_B \cdot N = \text{cst}$$



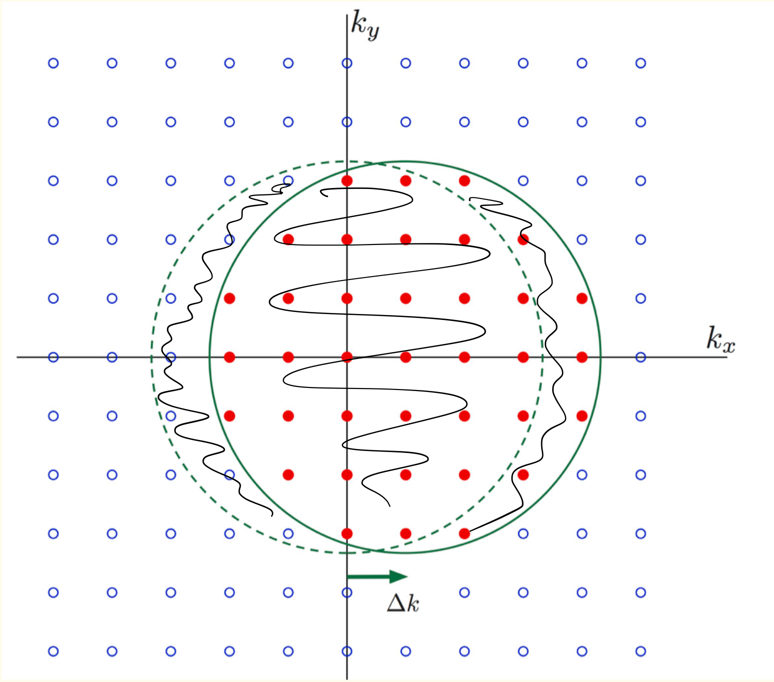
$$C = aT + bT^3$$

Conductivity

Scattering time τ

$$-eE_0\tau = \hbar\Delta k$$

$$\Delta k = \frac{-eE_0\tau}{\hbar}$$



J

$$N_J = \frac{\underline{4\pi k_F^2}\,\underline{\Delta k}}{\frac{4\pi}{3} k_F^3}\cdot \underline{N} \propto \frac{\Delta k}{k_F}\cdot N$$

$$\Delta k = \frac{-eE_0\tau}{\hbar} \qquad = -\frac{eE_0}{\hbar k_F}\,\tau N$$

$$J = -e\langle v\rangle N_J$$

$$\langle p/m\rangle \approx \frac{\hbar k_F}{m}$$

$$\frac{I}{V} = j = \underbrace{\frac{ne^2\tau}{m}}_{1/R = \sigma} E_0$$

$n = N/V$

Drude model

"$I = V/R$"

ne	charge density
e/m	acceleration
τ	scattering time

$$ne \frac{\Delta k}{\cancel{k_F}} \cdot \cancel{k_F} \cdot \tau$$

Tight-binding

H_2^+-molecule.

$$\hat H = \frac{\hat P_e^2}{2m} + \frac{e^2}{4\pi\varepsilon_0|R_L-R_R|} - \frac{e^2}{4\pi\varepsilon_0|R_L-\hat R_e|} - \frac{e^2}{4\pi\varepsilon_0|R_R-\hat R_e|}$$

$|L\rangle$

$|R\rangle$

$$\hat I = |L\rangle\langle L| + |R\rangle\langle R|$$

$$|\psi\rangle = \alpha|R\rangle + \beta|L\rangle$$

$$H = \begin{pmatrix} |R\rangle & |L\rangle \end{pmatrix} \begin{pmatrix} \langle R|\hat H|R\rangle & \langle R|\hat H|L\rangle \\ \langle L|\hat H|R\rangle & \langle L|\hat H|L\rangle \end{pmatrix} \begin{pmatrix} \langle R| \\ \langle L| \end{pmatrix}$$

$\hat I \hat H \hat I$

$$\langle R| \frac{p_e^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 |R_R - \hat{R}_e|} |R\rangle = E_0$$

$$\langle R| \quad '' \quad |L\rangle = 0$$

$$\langle R| \frac{-e^2}{4\pi |R_L - \hat{R}_e|} |R\rangle = \frac{-e^2}{4\pi\varepsilon_0} \int dr \frac{|\psi(r)|^2}{|R_L - r|}$$

ϕ

$$\psi(r) \simeq \delta(r - R_R)$$

$$= -\frac{e^2}{4\pi\varepsilon_0 |R_L - R_R|}$$

$$\langle L | \frac{-e^2}{4\pi\varepsilon_0 |R_L - \hat{R}_e|} | R \rangle = \frac{-e^2}{4\pi\varepsilon_0} \int dr \, \frac{\psi_L^*(L)\, \psi_R(r)}{|R_L - r|}$$

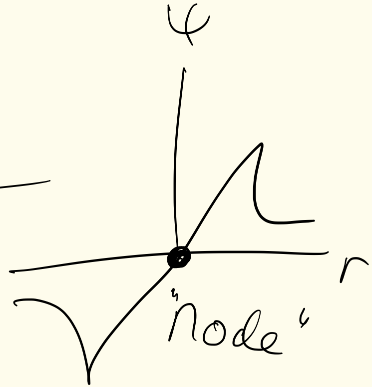
$$= -t$$

$$\Rightarrow \quad H = \begin{pmatrix} E_0 & -t \\ -t & E_0 \end{pmatrix}$$

$$= E_0 \left(\overline{c_R^\dagger c_R} + c_L^\dagger c_L \right) - t \left(c_L^\dagger c_R + c_R^\dagger c_L \right)$$

$$|\psi_0\rangle = \sqrt{\tfrac{1}{2}}\left(|L\rangle + |R\rangle\right)$$

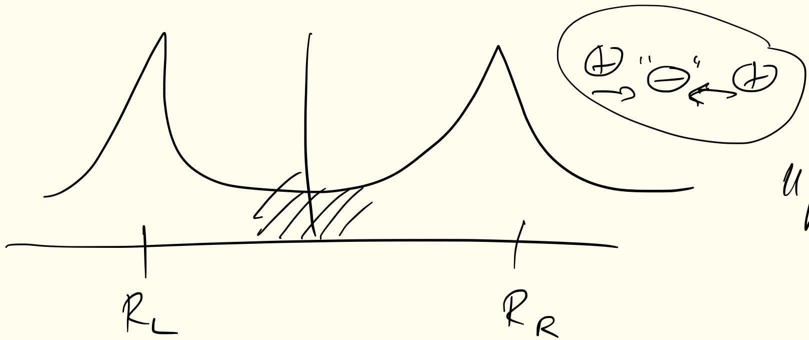
$$|\psi_1\rangle = \sqrt{\tfrac{1}{2}}\left(|L\rangle - |R\rangle\right)$$



"antibonding"

H_2^+

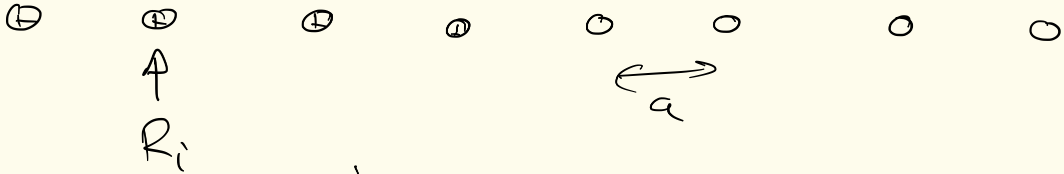
$\psi_0(r)$



"bonding"

Lecture 3C

1D)



$i = 1 \ldots N$

$|i\rangle$

$\hat{c}_i^\dagger$

$$\hat{H} = \sum_{i=1}^{N} E_0 \, \hat{c}_i^\dagger \hat{c}_i + \sum -t \, \hat{c}_i^\dagger \hat{c}_j$$

$$= \sum_{k} \left(E_0 - 2t \cos(ka) \right) \hat{c}_k^\dagger \hat{c}_k$$

L

$\Delta k = \frac{2\pi}{L}$

$L = Na$

$2\pi/L$

$-\pi/a$ $\quad k \quad$ π/a

a

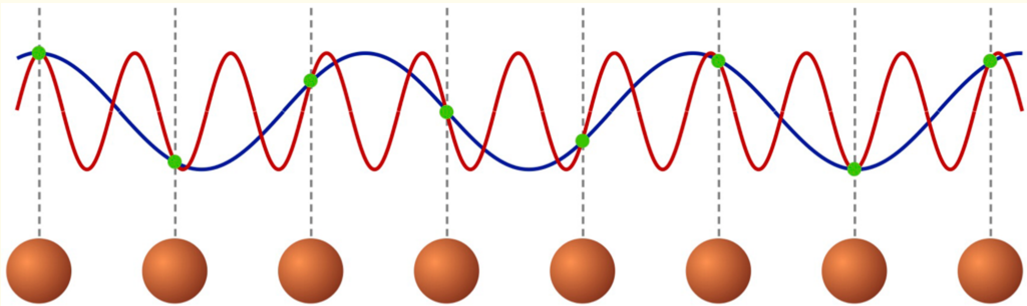
$R_i = i a$

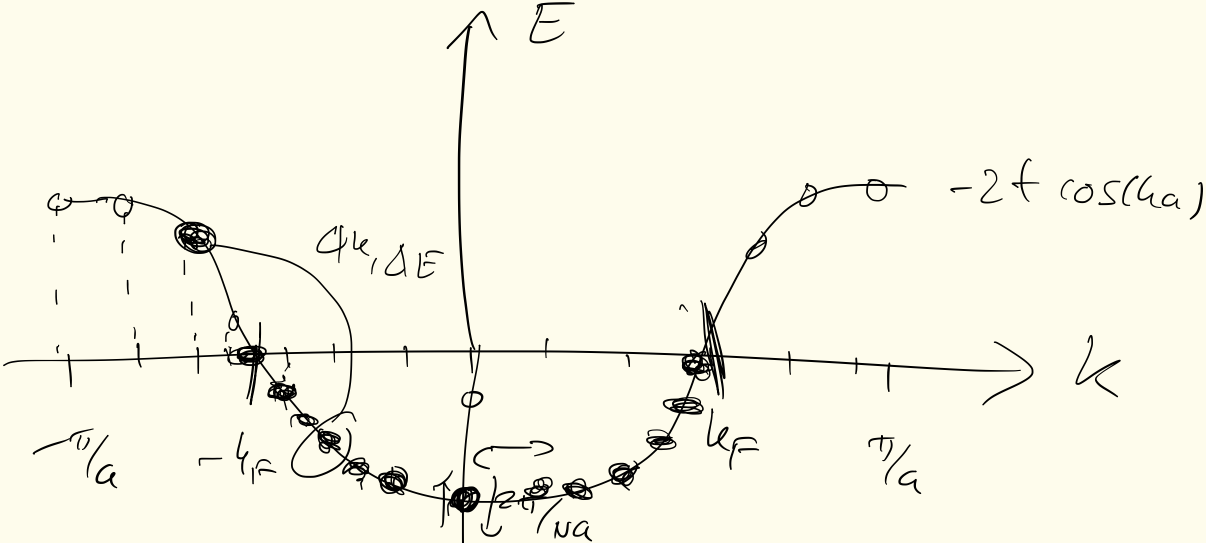
$i \in \cancel{\mathbb{Z}}\,[1, N]$

$-\pi/a \leq k < \frac{\pi}{a}$

first Brillouin zone

$\psi\left(k + \frac{2\pi}{a}\right) = \psi(k)$

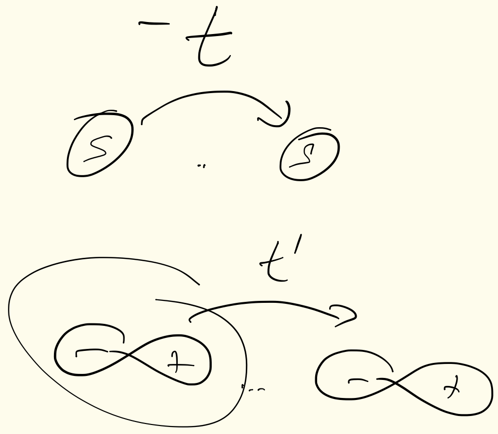




$1\, e^-/\text{atom}$

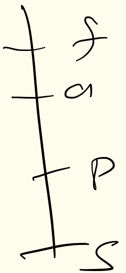
$\Rightarrow N e^-$

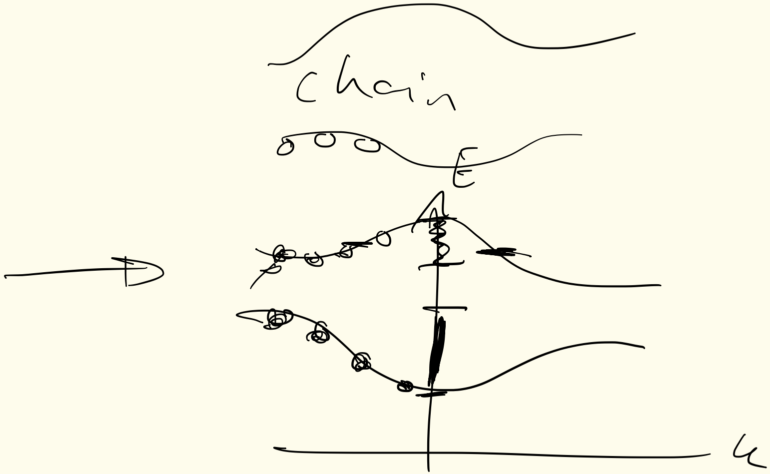
$$H = \sum_k \left(E_0 - 2t\cos(ka) \right) \hat{c}_k^\dagger \hat{c}_k$$



$$-\int \frac{\psi_L^* \psi_R}{r}$$

Hydrogen

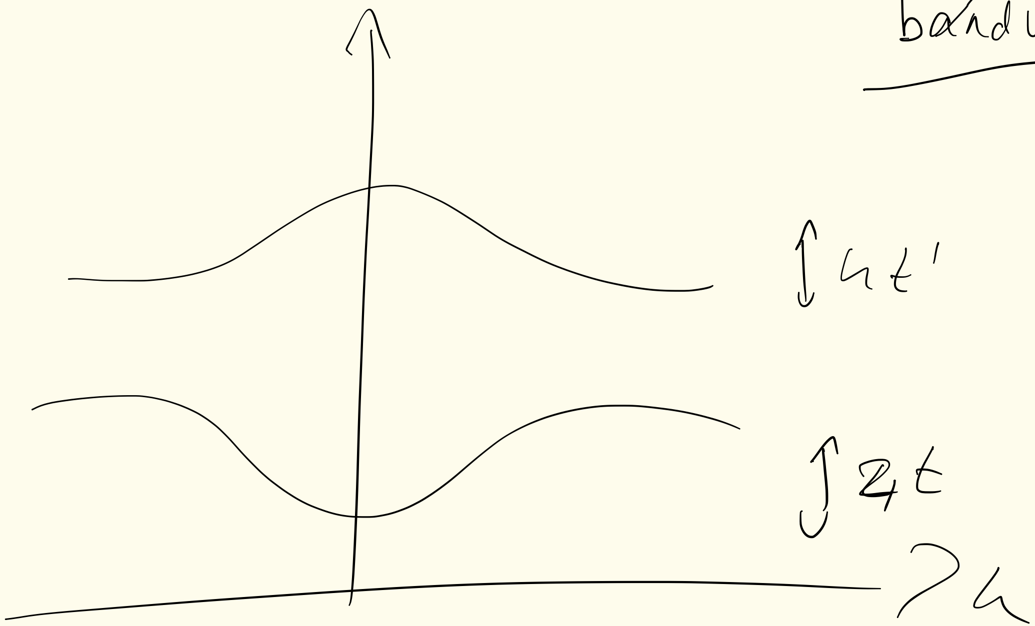


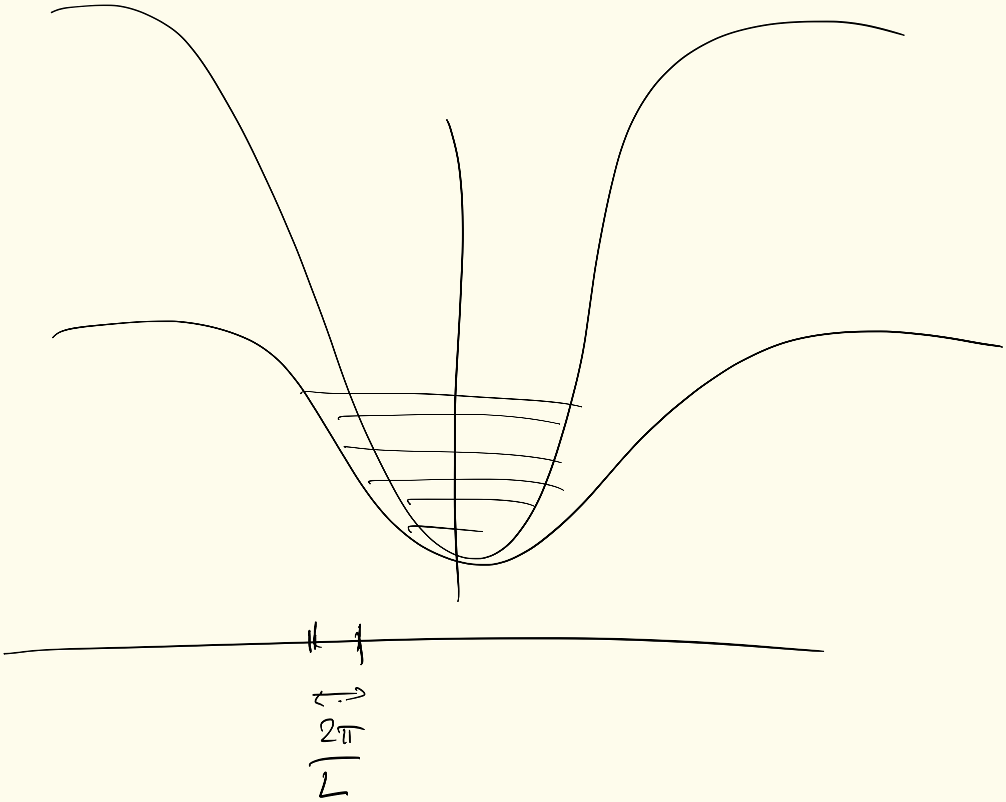


~~eng~~ energy bands

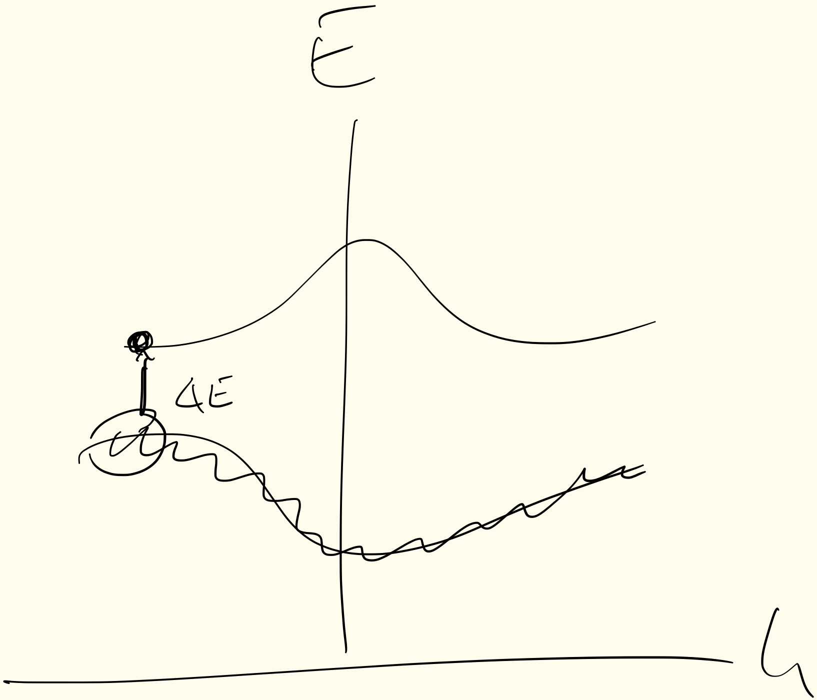
band structure

bandwidth





2π
L


E
ΔE
q

$i = n$

$j = m$

$$\sum_{ij} \rho_i \rho_j$$

$$\rho_i = \sum_{\sigma} c^{\dagger}_{i\sigma} c_{i\sigma}$$

$i = m$

$j = n$

$$\sum_{ij} c^{\dagger}_{i\sigma} c^{\dagger}_{j\sigma'} c_{i\sigma'} c_{j\sigma}$$

$$\sum_{ij} \rho_i \rho_j \Rightarrow U \sum_i \rho_i \rho_i = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$\boxed{H = -t \sum_{i\sigma} c^\dagger_{i\sigma} c_{i+1,\sigma} + U \sum_i \underline{n_{i\uparrow} n_{i\downarrow}}}$$

Hubbard

$\left.\begin{array}{l}\frac{1}{2}\text{ filling} \quad 1e^-/\text{atom} \\ U \to \infty\end{array}\right\}$ Mott – Hubbard

$\uparrow \quad \uparrow \quad \uparrow \quad \uparrow \quad \uparrow$

$-\dfrac{t^2}{U}$

$\Rightarrow \uparrow \quad \downarrow \quad \uparrow \quad \downarrow \quad \uparrow \quad \downarrow$

$-t\, c^\dagger_i c_{i+1} + U\, n_{i\uparrow} n_{i\uparrow}$

$$V \sum_{\langle ij \rangle} \rho_i \rho_j$$

Charge density waves

$$\sum_{\substack{ij \\ \sigma\sigma'}} V_{ij} \quad c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{i\sigma'} c_{j\sigma}$$

$$= -2V_{ij}\left(\vec{S}_i \cdot \vec{S}_j + \frac{1}{4}\rho_i \rho_j\right)$$

$$\hat{S}^+_i = c^\dagger_{i\uparrow} c_{i\downarrow}$$

$$\hat{S}^-_i = c^\dagger_{i\downarrow} c_{i\uparrow}$$

$$\hat{S}^z_i = \frac{1}{2}\left(c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow}\right)$$

$\Longrightarrow$ ferromagnet

$\uparrow\uparrow\uparrow\uparrow$