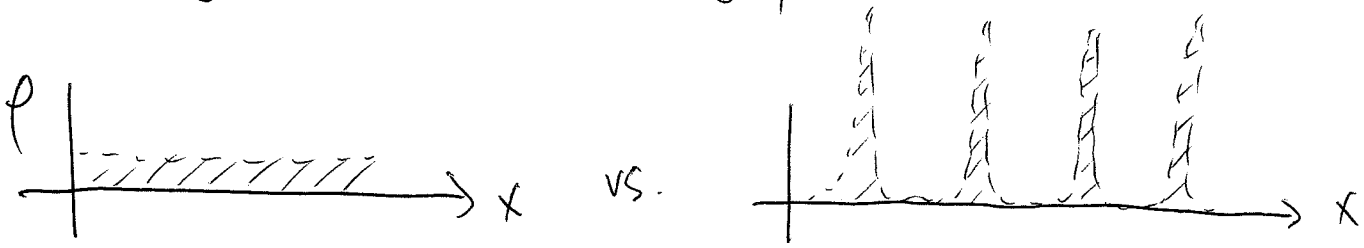
Phys 726 – Lecture 10

Solid State Systems

* We've considered jellium models in which the electronic charge is compensated by a smeared-out uniform background charge

* But in real materials, positive charge is not smoothly distributed; it is highly concentrated in the ionic cores of the constituent atoms

→ charge distribution is highly nonuniform

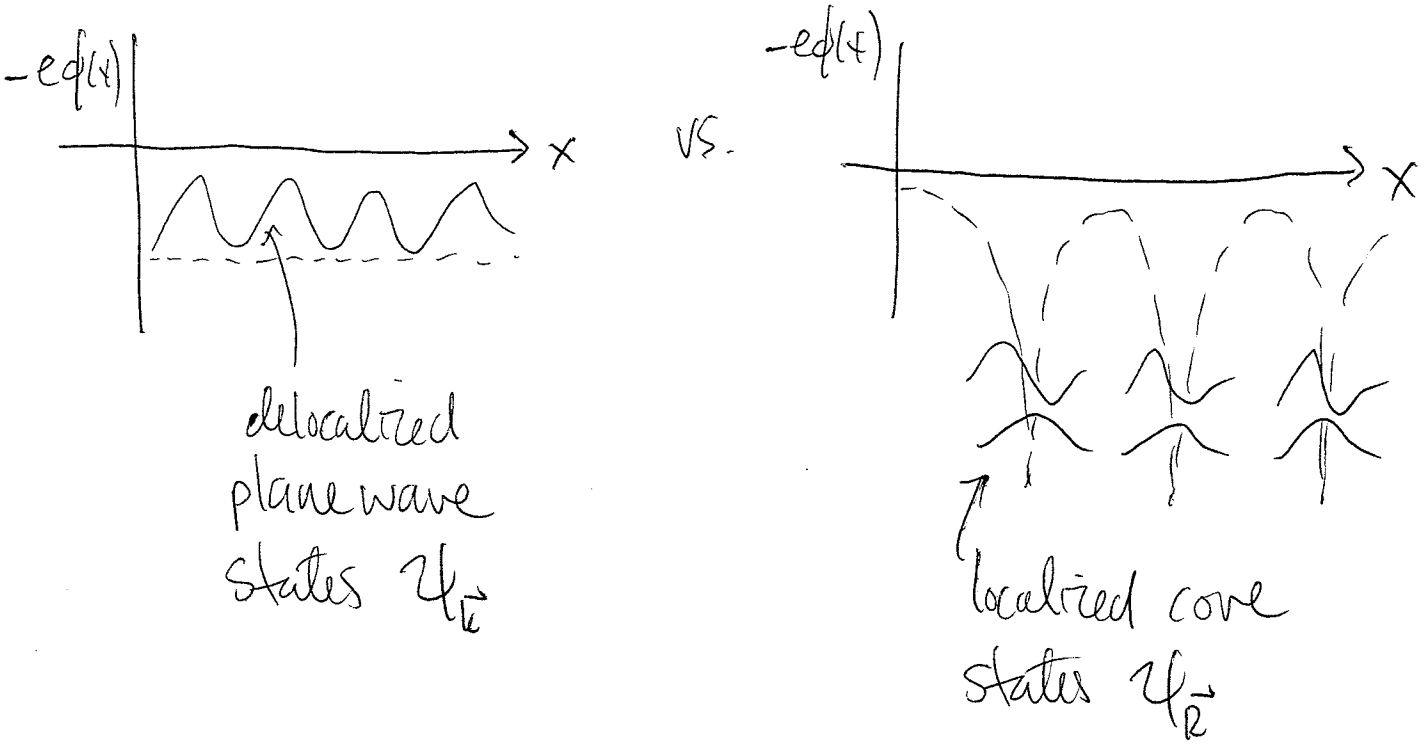


→ in regular solids, the distribution is periodic (i.e. it has a spatial modulation described by some wave vector $\vec{Q} \neq 0$)

→ electrons will feel an attractive potential

$$-e\phi(x) = -e\int dy \, \frac{\rho(y)}{|x-y|}$$

characterized by strongly negative divergences



$\Rightarrow$ deep wells may support many localized orbitals

$\rightarrow$ suppose that some set $\{\phi_{\vec{R},n}(\vec{r})\}$ spans the space of single-particle states

($\vec{R}$: atomic location; n: orbital index)

Then $\hat{\psi}_\alpha(\vec{r})$ has an expansion

$$\hat{\psi}_\alpha(\vec{r}) = \sum_{\vec{R}} \sum_{n} \phi_{\vec{R},n}(\vec{r})\, C_{\vec{R},n,\alpha}$$

$$= \sum_{\vec{R}} \sum_{n} \phi_n(\vec{r}-\vec{R})\, C_{\vec{R},n,\alpha}$$

NB for simplicity, we're taking all ions to be equivalent and the crystal basis to be trivial

* The noninteracting part of the Hamiltonian is

$$\hat{H}_0 = \sum_\alpha \int d^3r \, \hat{\psi}^\dagger_\alpha(\vec{r}) \, T(\vec{r}) \, \hat{\psi}_\alpha(\vec{r})$$

$$= \sum_\alpha \int d^3r \sum_{\vec{R}} \sum_n \phi^*_n(\vec{r}-\vec{R}) \, T(\vec{r}) \sum_{\vec{R}'} \sum_{n'} \phi_{n'}(\vec{r}-\vec{R}') \, c^\dagger_{\vec{R},n,\alpha} \, c_{\vec{R}',n',\alpha}$$

$$= \sum_\alpha \sum_{n,n'} \sum_{\vec{R}\vec{R}'} \int d^3r \, \phi^*_n(\vec{r}-\vec{R}) \, T(\vec{r}) \, \phi_{n'}(\vec{r}-\vec{R}') \, c^\dagger_{\vec{R},n,\alpha} \, c_{\vec{R}',n',\alpha}$$

$$= \int d^3r \, \phi^*_n(\vec{r}) \, T(\vec{r}) \, \phi_{n'}(\vec{r}+\vec{R}-\vec{R}')$$

$$\equiv -t_n(\vec{R}-\vec{R}') \, \delta_{nn'}$$

$$= -\sum_\alpha \sum_n \sum_{\vec{R}\vec{R}'} t_n(\vec{R}-\vec{R}') \, c^\dagger_{\vec{R},n,\alpha} \, c_{\vec{R}',n',\alpha}$$

$\longrightarrow$ system with discrete translational symmetry and hence <u>crystal momentum</u> eigenstates

$$c_{\vec{k},n,\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \, c_{\vec{R},n,\alpha}$$

$\vec{k}$: crystal momentum wave vector in BZ

N: number of atomic sites

→ inverse transformation

$$c_{\vec{R},n,\alpha} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+i\vec{k}\cdot\vec{R}} c_{\vec{k},n,\alpha}$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+i\vec{k}\cdot\vec{R}} \left(\frac{1}{\sqrt{N}} \sum_{\vec{R}'} e^{-i\vec{k}\cdot\vec{R}'} c_{\vec{R}',n,\alpha} \right)$$

$$= \frac{1}{N} \sum_{\vec{R}} \sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}-\vec{R}')} c_{\vec{R}',n,\alpha} = c_{\vec{R},n,\alpha} \quad \checkmark$$

$$\sum_{\vec{k}} e^{i\vec{k}\cdot(\vec{R}-\vec{R}')} = N\delta_{\vec{R},\vec{R}'}$$

→ diagonalize the Hamiltonian in k-space

$$\hat{H}_0 = -\sum_{\alpha} \sum_{n} \sum_{\vec{R},\vec{R}'} t_n(\vec{R}-\vec{R}')\, c^{\dagger}_{\vec{R},n,\alpha} c_{\vec{R}',n,\alpha}$$

$$= -\sum_{\alpha} \sum_{n} \sum_{\vec{R},\vec{R}'} t_n(\vec{R}-\vec{R}') \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{+i\vec{k}\cdot\vec{R}} c_{\vec{k},n,\alpha} \right)^{\dagger}$$

$$\times \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}'} e^{i\vec{k}'\cdot\vec{R}'} c_{\vec{k}',n,\alpha} \right)$$

$$= -\sum_{\alpha} \sum_{\vec{k},\vec{k}'} \sum_{n} \left(\frac{1}{N} \sum_{\vec{R},\vec{R}'} e^{-i\vec{k}\cdot\vec{R}} t_n(\vec{R}-\vec{R}') e^{+i\vec{k}'\cdot\vec{R}'} \right) \cdot c^{\dagger}_{\vec{k},n,\alpha} c_{\vec{k}',n,\alpha}$$

Let $\vec{R} \to \vec{R}'$ so that

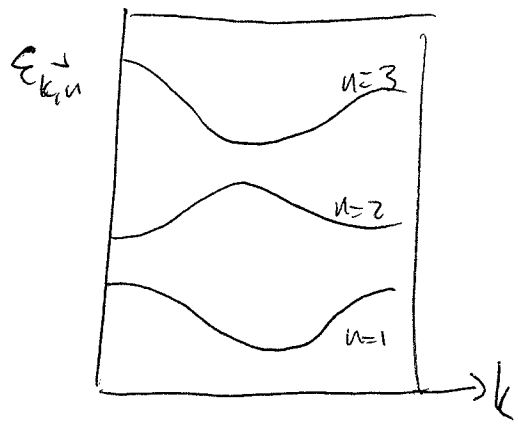
$$\frac{1}{N} \sum_{\vec{R}\vec{R}'} e^{-i\vec{k}\cdot(\vec{R}+\vec{R}')} t_n(\vec{R}) e^{+i\vec{k}'\cdot\vec{R}'}$$

$$= \underbrace{\frac{1}{N} \sum_{\vec{R}'} e^{i(\vec{k}'-\vec{k})\cdot\vec{R}'}}_{\equiv \delta_{\vec{k},\vec{k}'}} \cdot \underbrace{\sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} t_n(\vec{R})}_{\equiv -\varepsilon_{\vec{k},n}}$$

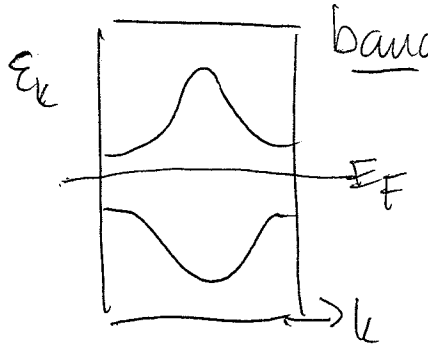
electronic dispersion for band n

i.e.

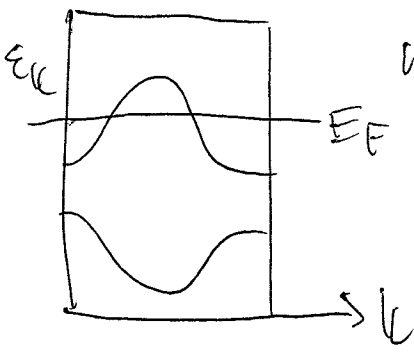
$$\hat{H}_0 = \sum_{\alpha} \sum_{k} \varepsilon_{\vec{k},n} c^{\dagger}_{\vec{k},n,\alpha} c_{\vec{k},n,\alpha}$$



* Recall the classification for noninteracting electrons



band insulator



metallic

* Interaction term

$$\hat{H}_1 = \frac{1}{2}\sum_{\alpha\beta}\int d^3r\, d^3r'\, \hat{\psi}^\dagger_\alpha(\vec{r})\,\hat{\psi}^\dagger_\beta(\vec{r}')\,V(\vec{r}-\vec{r}')\,\hat{\psi}_\beta(\vec{r}')\,\hat{\psi}_\alpha(\vec{r})$$

↑ by transl. invariance, $V(\vec{r}-\vec{r}')$

→ Substitute $\hat{\psi}_\alpha(\vec{r}) = \sum_{\vec{R}}\sum_{n} \phi_n(\vec{r}-\vec{R})\,c_{\vec{R},n,\alpha}$

$$\hat{H}_1 = \frac{1}{2}\sum_{\alpha\beta}\int d^3r\, d^3r' \left(\sum_{\vec{R}_1 n_1}\phi^*_{n_1}(\vec{r}-\vec{R}_1)\,c^\dagger_{\vec{R}_1 n_1\alpha}\right)$$

$$\times\left(\sum_{\vec{R}_2 n_2}\phi^*_{n_2}(\vec{r}'-\vec{R}_2)\,c^\dagger_{\vec{R}_2 n_2\beta}\right)$$

$$\times V(\vec{r}-\vec{r}')$$

$$\times\left(\sum_{\vec{R}_3 n_3}\phi_{n_3}(\vec{r}'-\vec{R}_3)\,c_{\vec{R}_3 n_3\beta}\right)$$

$$\times\left(\sum_{\vec{R}_4 n_4}\phi_{n_4}(\vec{r}-\vec{R}_4)\,c_{\vec{R}_4 n_4\alpha}\right)$$

$$= \frac{1}{2}\sum_{\alpha\beta}\sum_{\vec{R}_1\ldots\vec{R}_4}\sum_{n_1\ldots n_4} \int d^3r\, \phi^*_{n_1}(\vec{r}-\vec{R}_1)\,\phi_{n_4}(\vec{r}-\vec{R}_4)$$

$$\cdot\int d^3r'\,\phi_{n_2}(\vec{r}'-\vec{R}_2)\,\phi_{n_3}(\vec{r}'-\vec{R}_3)\,V(\vec{r}-\vec{r}')$$

$$\cdot c^\dagger_{\vec{R}_1 n_1\alpha}\,c^\dagger_{\vec{R}_2 n_2\beta}\,c_{\vec{R}_3 n_3\beta}\,c_{\vec{R}_4 n_4\alpha}$$

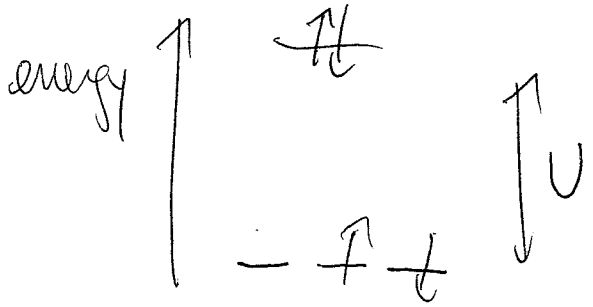
→ simplify by ignoring the band index and assuming that the potential is short-ranged: $V \approx U\delta(\vec{r}-\vec{r}')$

$$\hat{H}_1 = U \sum_{\alpha<\beta} \sum_{R} c^{\dagger}_{R\alpha} c^{\dagger}_{R\beta} c_{R\beta} c_{R\alpha}$$

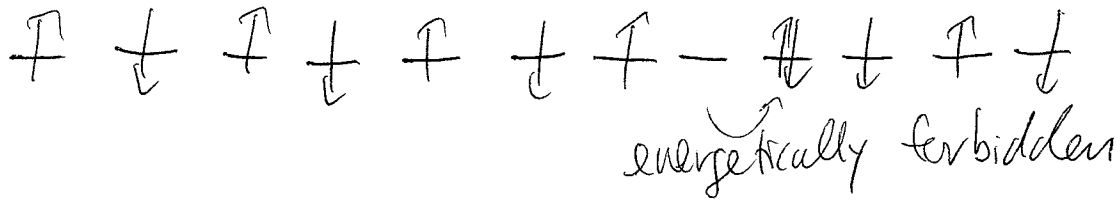
$$= U \sum_{\vec{R}} c^{\dagger}_{R\uparrow} c_{R\uparrow} \cdot c^{\dagger}_{R\downarrow} c_{R\downarrow}$$

$$= U \sum_{\vec{R}} \hat{n}_{\vec{R}\uparrow} \hat{n}_{\vec{R}\downarrow}$$

↑ penalizes double occupancy

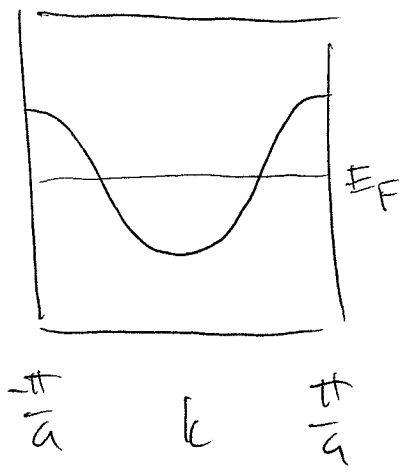


→ near half-filling, the electrons become locked into place in the large-U limit

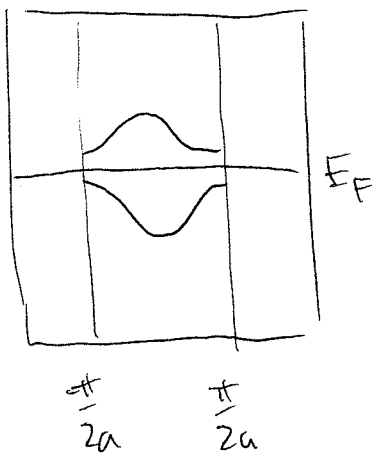


* We'll show next class that the residual interactions $O(t^2/U)$ favour antiferromagnetic alignment of the localized spins

small U



large U



- bands backfolded by $Q = \frac{\pi}{a}$
- interactions open up a gap of order t^2/U
- Mott insulator, rather than a band insulator