Bloch Theorem and Electron Bands

Note: reading chapters 8 + 9

- Assume: noninteracting electrons, simple product states.

$$\Psi = \psi_1(r_1)\psi_2(r_2)\psi_3(r_3)\ldots \qquad E = \sum_i \varepsilon_i$$

- Also Born-Oppenheimer approximation, and assume crystal potential includes average of all other electron interactions. (Hartree approximation)
- Justification comes later (Landau theory, ch. 17).
- Then can show, Bloch theorem form of wavefunction.

$$\psi_i = \sum_k \alpha_k e^{i\vec{k}\cdot\vec{r}} \qquad U(\vec{r}) = \sum_K U_{\vec{K}} e^{i\vec{K}\cdot\vec{r}}$$

U with crystal symmetry; ψ with periodic boundary conditions.

$$\rightarrow \sum_k e^{i\vec{k}\cdot\vec{r}} \left\{ \left(\frac{\hbar^2 k^2}{2m} - \varepsilon \right) \alpha_k + \sum_K U_K \alpha_{k-K} \right\} = 0$$

Schrödinger equation

$$\rightarrow \psi_i = u(\vec{r}) e^{i\vec{k}\cdot\vec{r}} = \left(\sum_K \alpha_{k,K} e^{i\vec{K}\cdot\vec{r}} \right) e^{i\vec{k}\cdot\vec{r}}$$

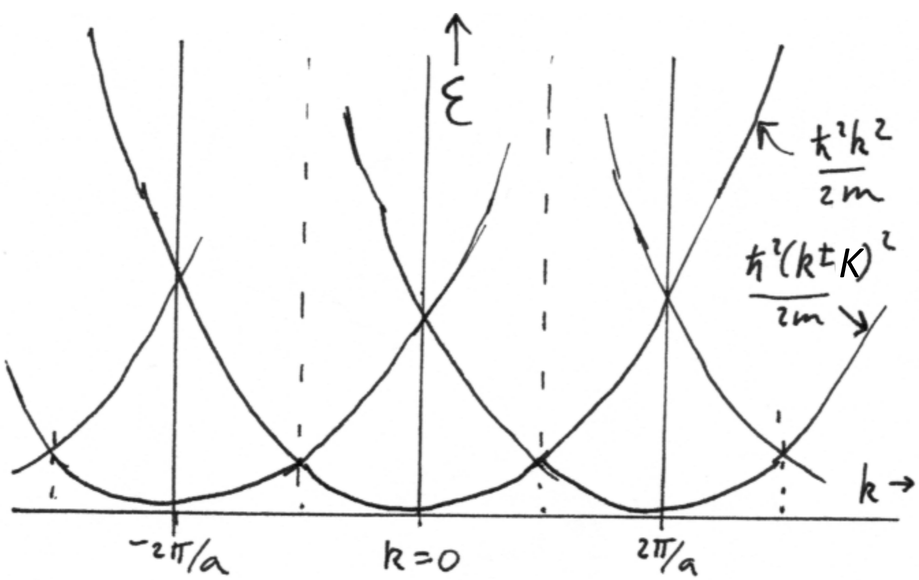
Bloch form (general form of wavefunction)

$$u(\vec{r}) = u(\vec{r} + \vec{R})$$

Bloch States and Electron Bands

- ❖ Can <u>always</u> re-define states by replacing $\vec{k}$ by $\vec{k} \pm \vec{K}$.
- ❖ Consequences: *k* over-determined modulo *K*; shows that *k* can be defined within <u>single Brillouin Zone</u>; *k* conservation rather than overall momentum. [*k* = "Crystal momentum"]

Free-electron states



- Note, each state is displayed multiple times in the figure.
- States appear <u>once</u> in each Brillouin Zone. [Twice with <u>spin</u>.]

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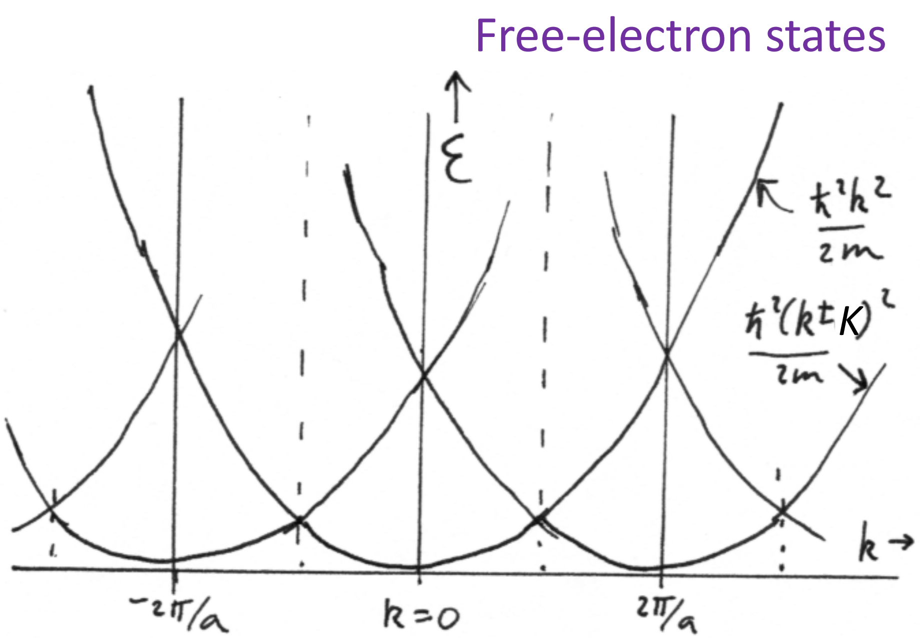

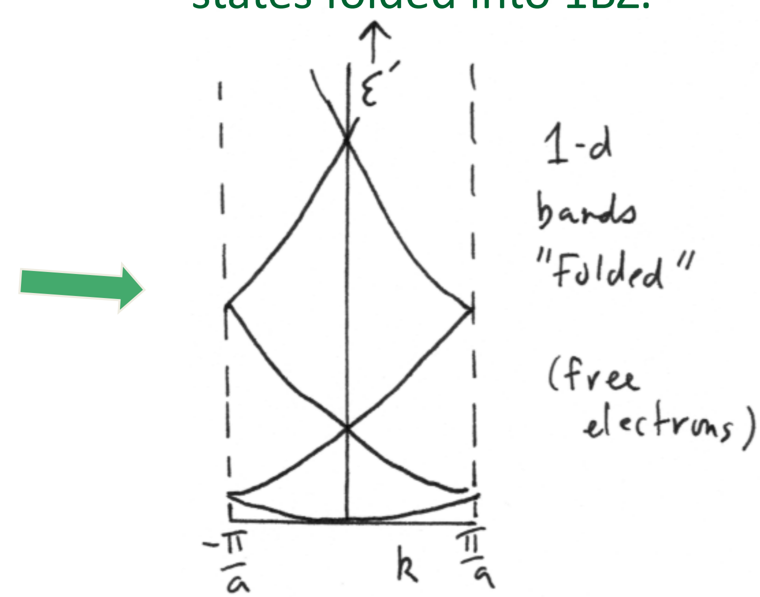

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Electrons with a crystal potential:

- Electron energies (and wavefunctions) no longer same as simple plane wave states; strongest effects at zone boundaries.
- Shown is typical case for small periodic potential ("nearly free electron model").

Free-electron states folded into 1BZ.