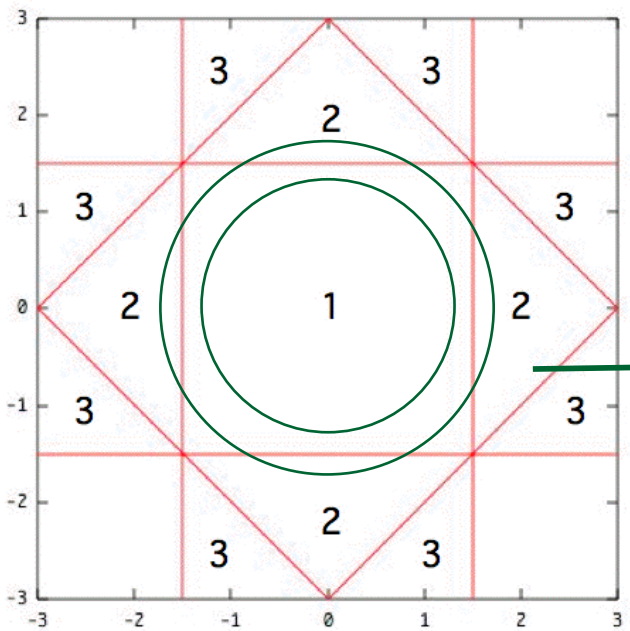
Electrons bands in 2D:

- Free electron Fermi surfaces are circles, area ∝ number of electrons.
- Square lattice example



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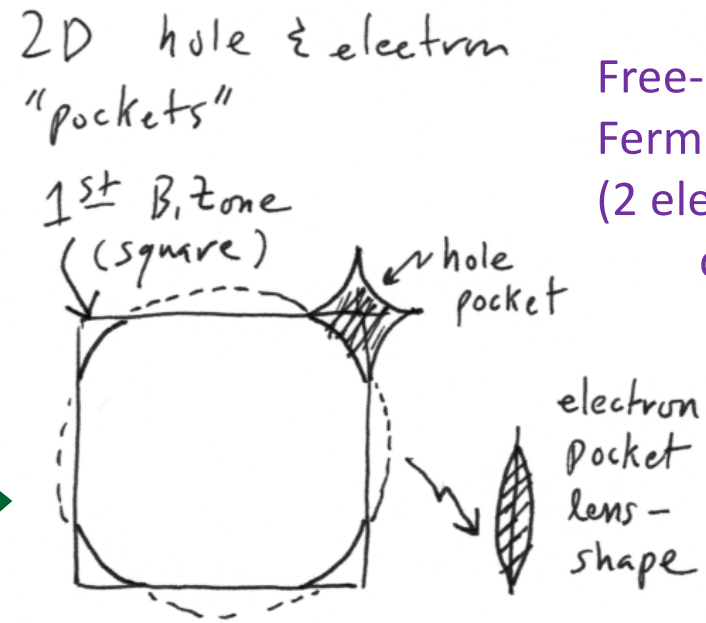


Free-electron Fermi surfaces (2 electrons/ cell)

- Folded → electron & hole pockets.
- With crystal potential: pockets will <u>shrink</u>.
- Larger potential → <u>insulator.</u>

Bloch theorem: electronic states for general crystal potential.

- Hamiltonian including periodic crystal potential

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + U(\vec{r})$$

← Actually summed over coordinates for each electron; solution is product wavefunction. (Assuming no e-e interactions.)

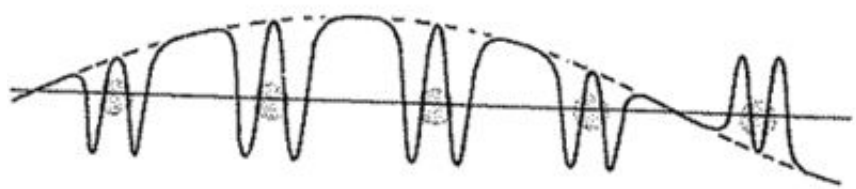
- Potential has Bravais lattice translation symmetry.

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

- Bloch theorem: Solutions of the above consist of plane wave multiplied by function with lattice symmetry.

(× a spin state; assume no spin-orbit coupling.)

$$\boxed{\psi(\vec{r}) = u(\vec{r})e^{i\vec{k}\cdot\vec{r}}}$$



$u(\vec{r}) = u(\vec{r} + \vec{R})$ $\vec{k}$ by periodic B.C.

Bloch theorem:

Assume $N_1 N_2 N_3$ cells. $$\vec{k} = \sum \frac{n_i}{N_i} \vec{b}_i$$ Note this fills <u>all</u> k space

Most general function with periodic B.C.: $$\psi = \sum_k \alpha_k e^{i\vec{k}\cdot\vec{r}}$$

Fourier theorem

Potential has symmetry: $$U(\vec{r}) = \sum_G U_G e^{i\vec{G}\cdot\vec{r}}$$

Fourier theorem for <u>crystal symmetric</u> function

$$H\psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + U(\vec{r})\psi = E\psi$$ Expand:

Bloch theorem:

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$$H\psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + U(\vec{r})\psi = E\psi$$

Expand:

$$\frac{\hbar^2}{2m}\sum_k \alpha_k k^2 e^{i\vec{k}\cdot\vec{r}} + \sum_{k,G} U_G \alpha_k e^{i(\vec{G}+\vec{k})\cdot\vec{r}} = E\sum_k \alpha_k e^{i\vec{k}\cdot\vec{r}}$$

Bloch theorem:

$$H\psi = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + U(\vec{r})\psi = E\psi$$

Expand:

$$\frac{\hbar^2}{2m}\sum_k \alpha_k k^2 e^{i\vec{k}\cdot\vec{r}} + \underbrace{\sum_{k,G} U_G \alpha_k e^{i(\vec{G}+\vec{k})\cdot\vec{r}}}_{\sum_{k,G} U_G \alpha_{k'-G} e^{i(\vec{k}')\cdot\vec{r}}} = E\sum_k \alpha_k e^{i\vec{k}\cdot\vec{r}}$$

k, k' dummy indices

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$$\sum_k e^{i\vec{k}\cdot\vec{r}}\left\{\left(\frac{\hbar^2 k^2}{2m} - E\right)\alpha_k + \sum_G U_G \alpha_{k-G}\right\} = 0$$

- To be true all r, curly bracket term must = 0 all k.
- Result <u>couples states k to $k \pm G$ only</u>.

Bloch theorem:

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- Result <u>couples states k to $k \pm G$ only</u>.
- Solution is a sum of $k \pm G$ <u>states</u>:

$$\psi = \underbrace{\left(\sum_G \alpha_{k,G} e^{i\vec{G}\cdot\vec{r}}\right)}_{\equiv u(\vec{r})} e^{i\vec{k}\cdot\vec{r}}$$

Lattice symmetry.
Theorem proved.

Note, can always re-configure k to $k + G'$

Bloch theorem:

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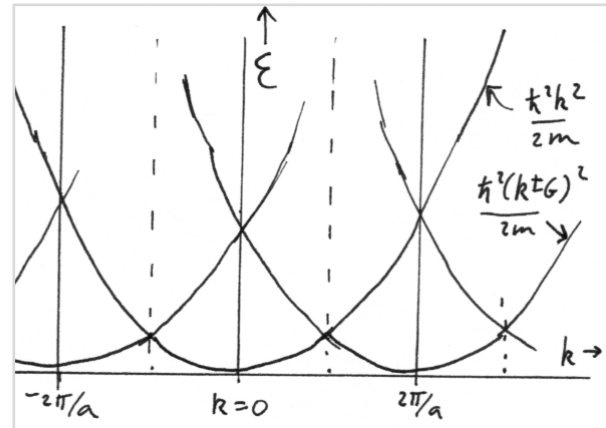

- Result couples states k to $k \pm G$ only.
- Solution,

$$\psi = \underbrace{\left(\sum_G \alpha_{k,G} e^{i\vec{G}\cdot\vec{r}}\right)}_{\equiv u(\vec{r})} e^{i\vec{k}\cdot\vec{r}}$$

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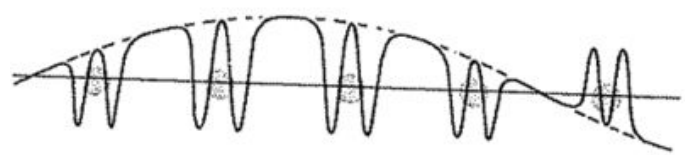

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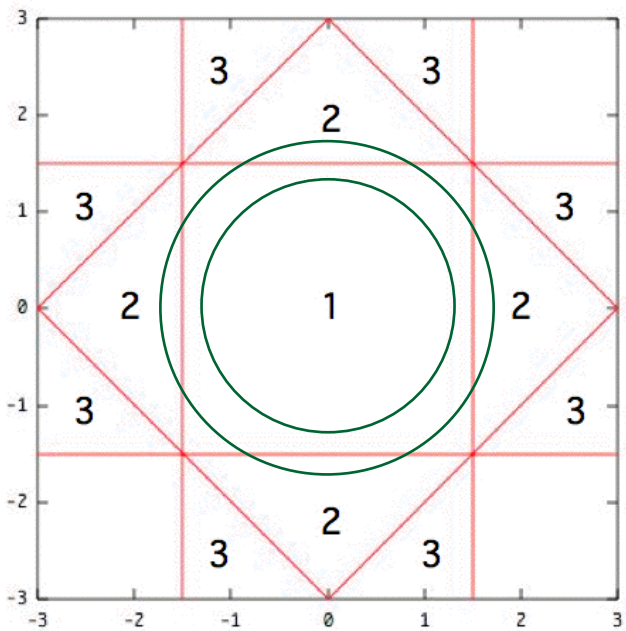

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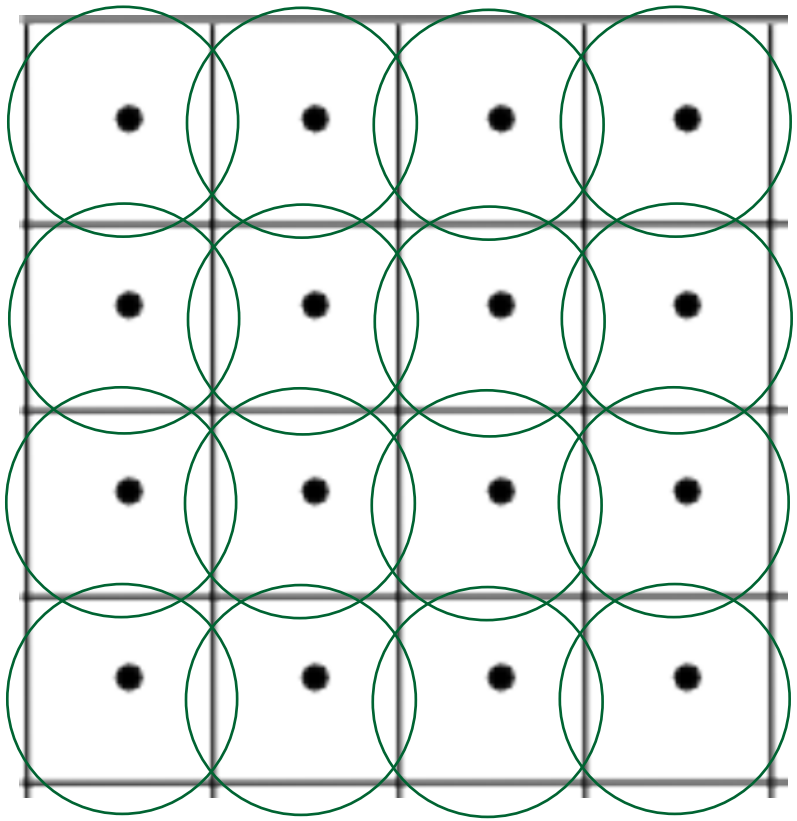

Fermi surfaces in “repeated-zone scheme”

Nearly-Free electron model:

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

Recall, $$U(\vec{r}) = \sum_G U_G e^{i\vec{G}\cdot\vec{r}}$$

$$\psi = \left(\sum_G \alpha_{k,G} e^{i\vec{G}\cdot\vec{r}} \right) e^{i\vec{k}\cdot\vec{r}}$$

Assume *U* <u>weak</u>; wavefunctions ≈ <u>plane waves</u>, $\varepsilon_o(k) \equiv \frac{\hbar^2 k^2}{2m}$

Perturbation through <u>2nd order</u>:

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + \sum_G \frac{|U_G|^2}{\varepsilon_o(\vec{k}) - \varepsilon_o(\vec{k} - \vec{G})}$$

- ❑ Uses result from before, U joins only states $k \pm G$.
- ❑ Small energy changes occur except when states are <u>degenerate</u>.
- ❑ Degeneracies: Bands always cross <u>on Brillouin Zone Boundaries</u>.
- ❑ (also sometimes *accidental* crossings).

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Assume *U* <u>weak</u>; wavefunctions ≈ <u>plane waves</u>, $\varepsilon_o(k) \equiv \dfrac{\hbar^2 k^2}{2m}$

Degenerate case: assume situation where only 2 states cross;

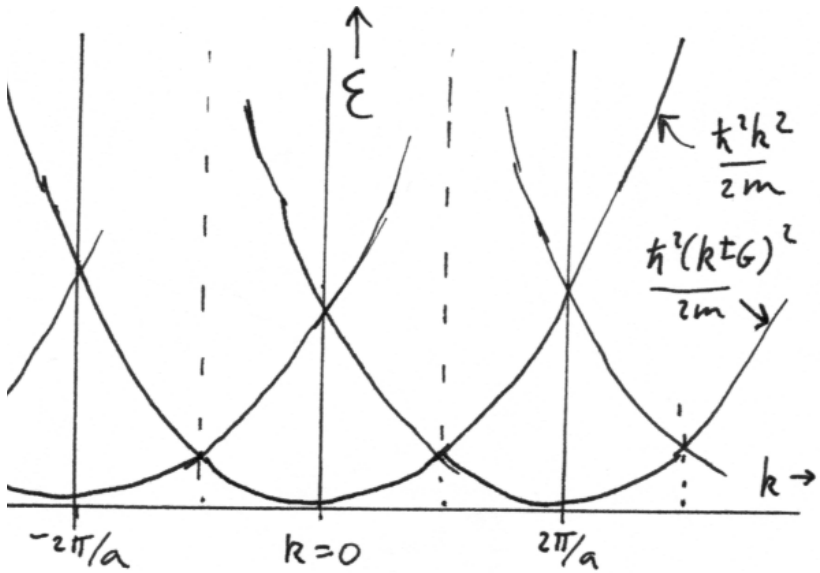
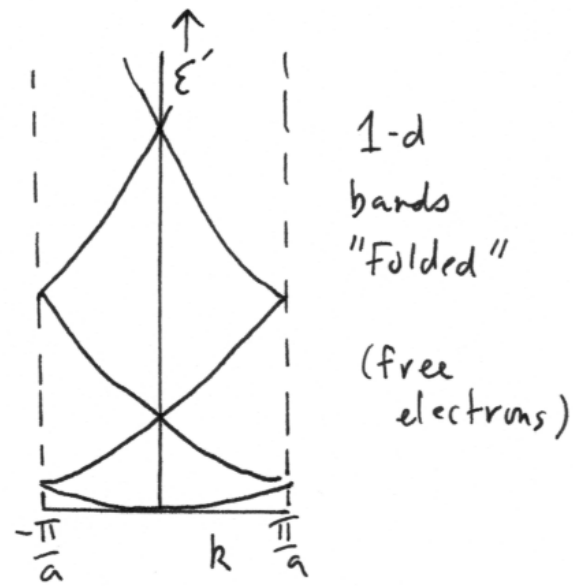
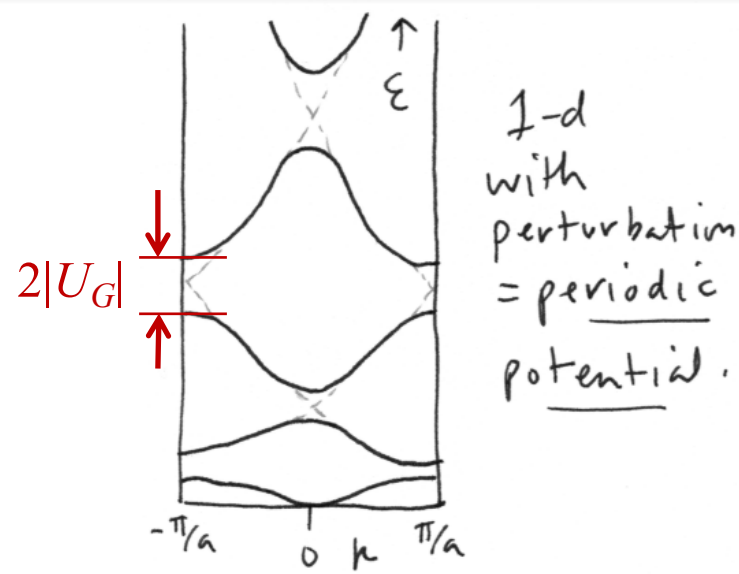
$$\frac{\hbar^2 k^2}{2m} \approx \frac{\hbar^2 (k-G)^2}{2m}$$ so can show, diagonalize 2×2 system:

$$\begin{pmatrix} \hbar^2 k^2/2m & U_G \\ U_{-G} & \hbar^2 (k-G)^2/2m \end{pmatrix} \cdot \begin{pmatrix} \alpha_k \\ \alpha_{k-G} \end{pmatrix} = \varepsilon \begin{pmatrix} \alpha_k \\ \alpha_{k-G} \end{pmatrix}$$

energy $\varepsilon_o \pm |U_G|$ at gap.

Results: States always have avoided crossing, gap = $2|U_G|$.

General solution shown in Mathematica notebook.

Nearly-free electrons:

Free-electron states, Extended zone scheme folded into 1BZ.