Nearly-Free electron model from last time: (Chapter 9 in text)

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

Bloch states

Assume *U* <u>weak</u>; perturbation theory $\varepsilon_o(k) \equiv \frac{\hbar^2 k^2}{2m}$

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

$$\varepsilon = \frac{\hbar^2 k^2}{2m} + \sum_K \frac{|U_K|^2}{\varepsilon_o(\vec{k}) - \varepsilon_o(\vec{k} - \vec{K})}$$

Recall, expansion breaks down on <u>zone</u> <u>boundaries</u>

Degenerate case: assume only 2 states cross; diagonalize 2×2 system.

A&M notation c_k

$$\frac{\hbar^2 k^2}{2m} \approx \frac{\hbar^2 (k-K)^2}{2m} \rightarrow \begin{pmatrix} \hbar^2 k^2 / 2m & U_K \\ U_{-K} & \hbar^2 (k-K)^2 / 2m \end{pmatrix} \cdot \begin{pmatrix} \alpha_k \\ \alpha_{k-K} \end{pmatrix} = \varepsilon \begin{pmatrix} \alpha_k \\ \alpha_{k-K} \end{pmatrix}$$

Avoided crossing, gap = $2|U_K|$ (to 1st order order in *U*)

General solution [Mathematica]:

```
(*  Nearly-free Hamiltonian for 2 states crossing  *)
Clear[k, uK]; MatrixForm[{{k^2, uK}, {uK, (k - 2 * Pi) ^2}}]
```

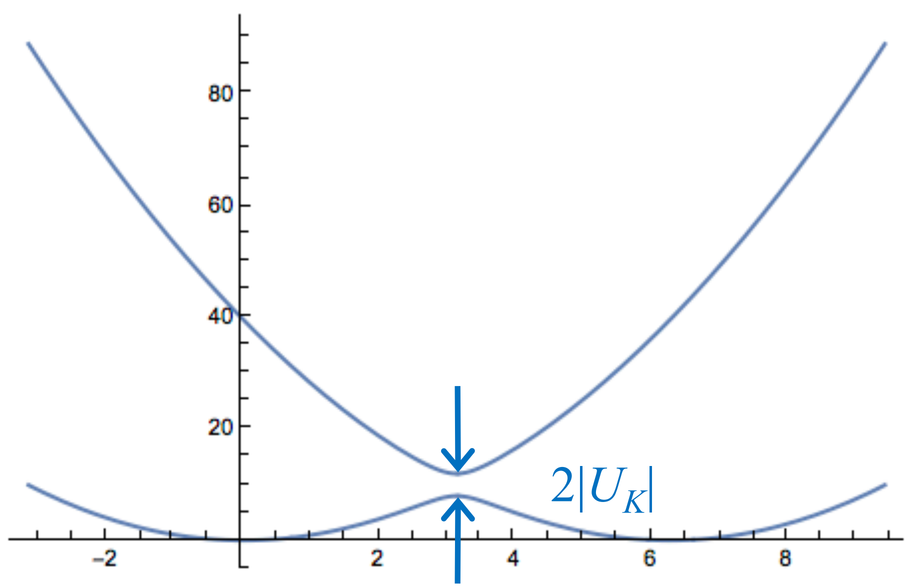
rixForm=

$$\begin{pmatrix} k^2 & uK \\ uK & (k-2\pi)^2 \end{pmatrix}$$

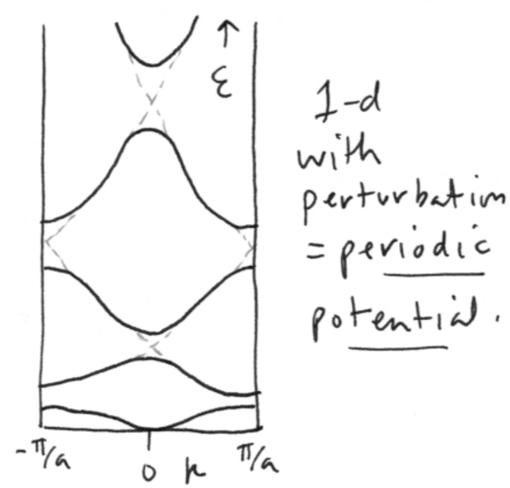
```
Clear[k, uK]; FullSimplify[Eigenvalues[{{k^2, uK}, {uK, (k - 2 * Pi) ^2}}]]
```

$$\left\{k^2 - 2 k \pi + 2 \pi^2 - \sqrt{4 (k-\pi)^2 \pi^2 + uK^2},\ k^2 - 2 k \pi + 2 \pi^2 + \sqrt{4 (k-\pi)^2 \pi^2 + uK^2}\right\}$$

```
uK = 2;
Plot[Eigenvalues[{{k^2, uK}, {uK, (k - 2 * Pi) ^2}}], {k, -1 * Pi, 3 * Pi}]
```



My sketch:

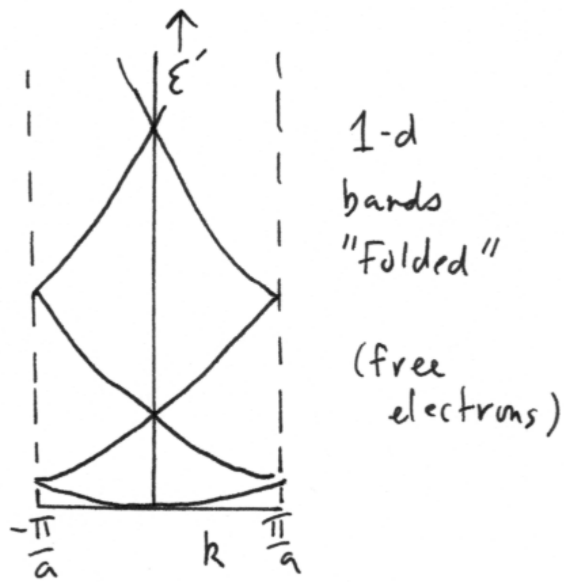


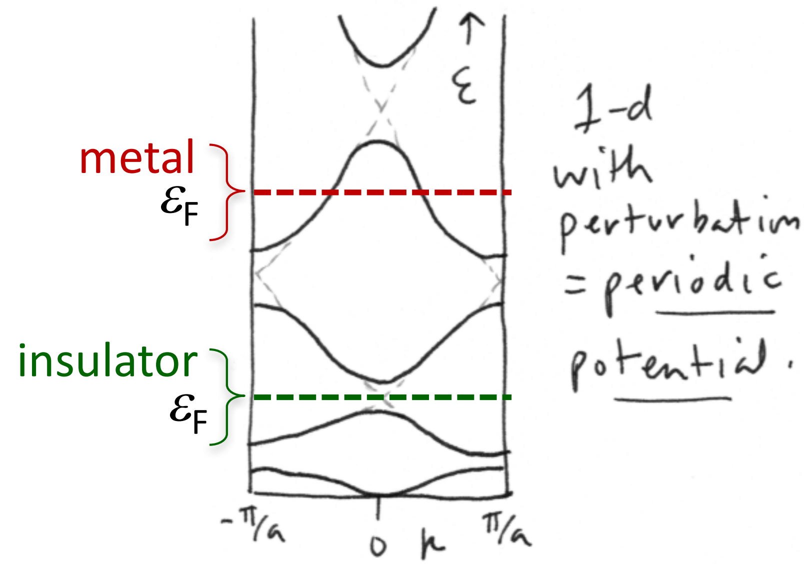
Electrons with a crystal potential:

Recall, 2*N* Bloch states (with spin) fit into a single Brillouin zone

(per band, before folding into 1st zone)

Free-electron
states folded into 1BZ.

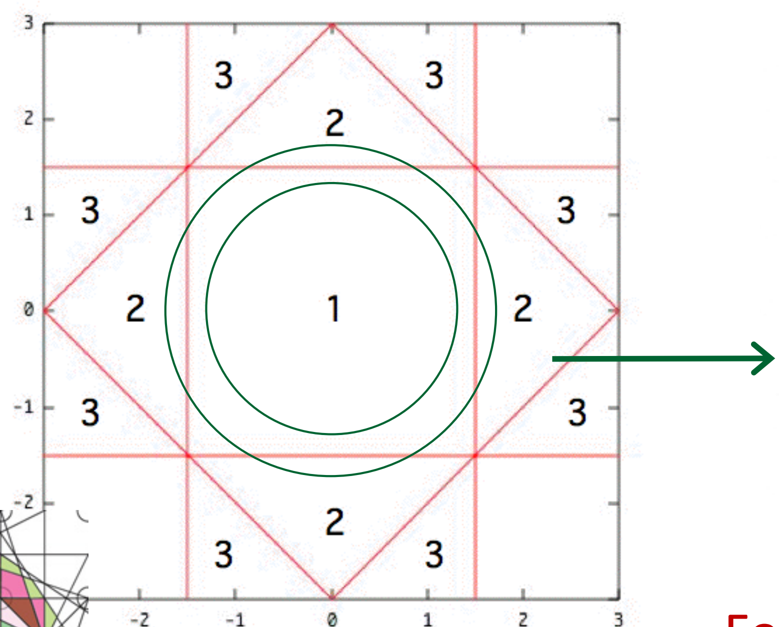




- notation, N = # cells in crystal.
- Even electron number per cell: insulator (simplest case).

Electrons bands in 2D:

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



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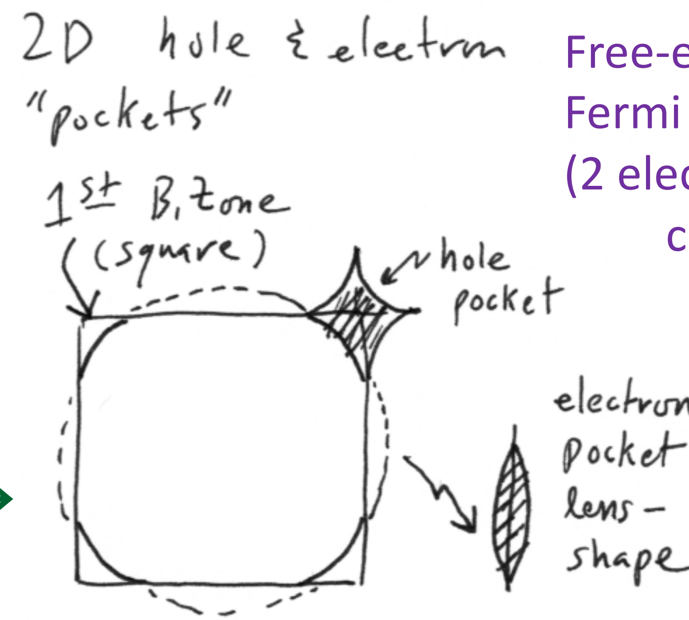
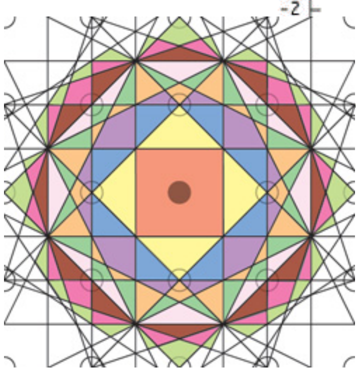


Free-electron Fermi surfaces (2 electrons/cell)



2D square
http://www.doitpoms.ac.uk/tlplib/brillouin_zones/index.php

Folded gives electron & hole pockets.
With $U \neq 0$: pockets will shrink.
2-electron: insulator if U large enough.