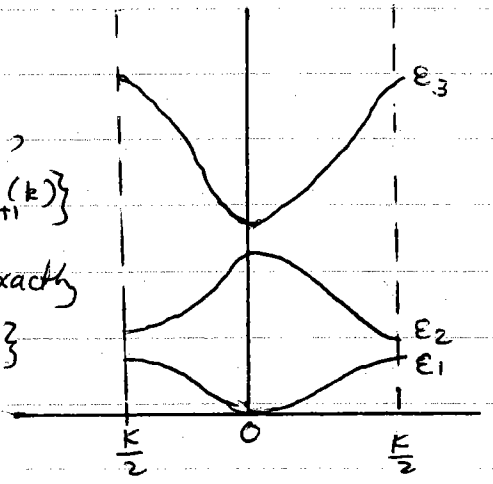
Ground state of electron gas in periodic potential

Fill up lowest energy single electron energy levels, to get lowest energy many electron state consistant with Pauli exclusion principle.

Each band can hold $2N$ electrons where N = # sites in B.L
- 2 ← # $\vec{k}$ states allowed
- spin up or spin down

⇒ each band can hold 2 electrons per Bravais lattice site

Example 1-d crystal – weak potential



in this model,
$\max\{\varepsilon_n(k)\} < \min\{\varepsilon_{n+1}(k)\}$
$\max\{\varepsilon_n\}$ lies exactly below $\min\{\varepsilon_{n+1}\}$
⇒ direct gap
$K = \frac{2\pi}{a}$

assume for simplicity, we have crystal structure with one ion on each B.L site, with valence Z. i.e. each B.L site gives Z conduction electrons

① If Z is even, then we completely fill up the lowest $Z/2$ bands, + all other bands empty.

② If Z is odd, then completely fill up lowest $\frac{Z-1}{2}$ bands, the next highest band is 1/2 filled, and all others are empty.

Case ① Z even : Material is insulator

Reason: In equilibrium, bands completely filled ⇒ there is an energy gap E_g to first excited state ($E_g = \min E_{\frac{Z}{2}+1} - \max$

⇒ unless electrons somehow receive an energy $\geq E_g$, they cannot scatter anywhere – no empty states to scatter to with energy smaller than E_g.
At low T, $k_B T \ll E_g$
If apply small electric field $\vec{E}$, it will not be able to scatter electrons and create a non-equilibrium state carrying a finite current (in equilib current = 0.
⇒ insulator

(Another way: we soon will see that the Bloch electron state ψ_{nk} has average velocity $\vec{v}_{nk} = \frac{\partial E_{nk}}{\hbar \partial k}$ (like group vel
For a filled band, the net velocity of all electrons sums to zero)

When $k_B T \gtrsim E_g$, the equilibrium state will have some electrons in excited states, i.e. some electrons are excited over the gap E_g from the $(Z/2)$ band into the $(\frac{Z}{2}+1)$ band – these can scatter and give rise to electric current.

⇒
- $k_B T \ll E_g$ ⇒ insulator
- $k_B T \gtrsim E_g$ ⇒ semiconductor # carriers $\sim e^{-E_g/k_B T}$

Case ② Z: odd : Material is metal

Reason: the highest band containing electrons, is partially (half) filled ~~even~~ at $T=0$.

⇒ at any T, there are empty states to scatter to with energy arbitrarily close to E_F ie no energy gap to lowest excited state

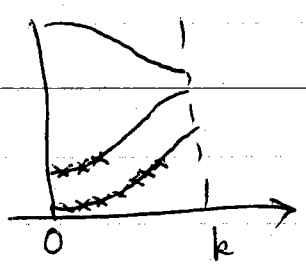
⇒ apply $\vec{E}$ can set up current carrying non-equilib distribution

So for 1-d weak potential, Z odd ⇒ metal
Z even ⇒ insulator

* For 2-d or 3-d weak potential (or even perhaps 1-d when potential is not weak) we will see that we in general do not have the case that

$$\max_k \{\varepsilon_n(k)\} < \min_k \{\varepsilon_{n+1}(k)\}$$

So that bands overlap. Then, even if Z is even, it may happen that we have several partially filled bands containing the most energetic electrons ⇒ metal



if $Z=2$

So Z even does not necessarily mean insulator
However insulator ~~does~~ still does require only completely filled bands ie Z even
⇒ Z even necessary but not sufficient for insulator

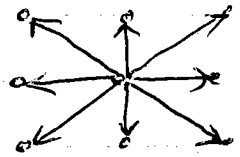
Band structure in 2-d — simple square Bravais lattice

R.L. is also square

$\vec{K} = K(n\hat{x} + m\hat{y})$ n, m integer $K = \frac{2\pi}{a}$

a = lattice const of B.L.

The smallest R.L. vectors are



$\vec{K}_0 = 0$

smallest $\{\vec{K}_1\} = \{\hat{x}, -\hat{x}, \hat{y}, -\hat{y}\}$ 4 choices

ext smallest $\{\vec{K}_2\} = \{K(\hat{x}+\hat{y}), K(\hat{x}-\hat{y}), K(-\hat{x}+\hat{y}), K(-\hat{x}-\hat{y})\}$ 4 choics

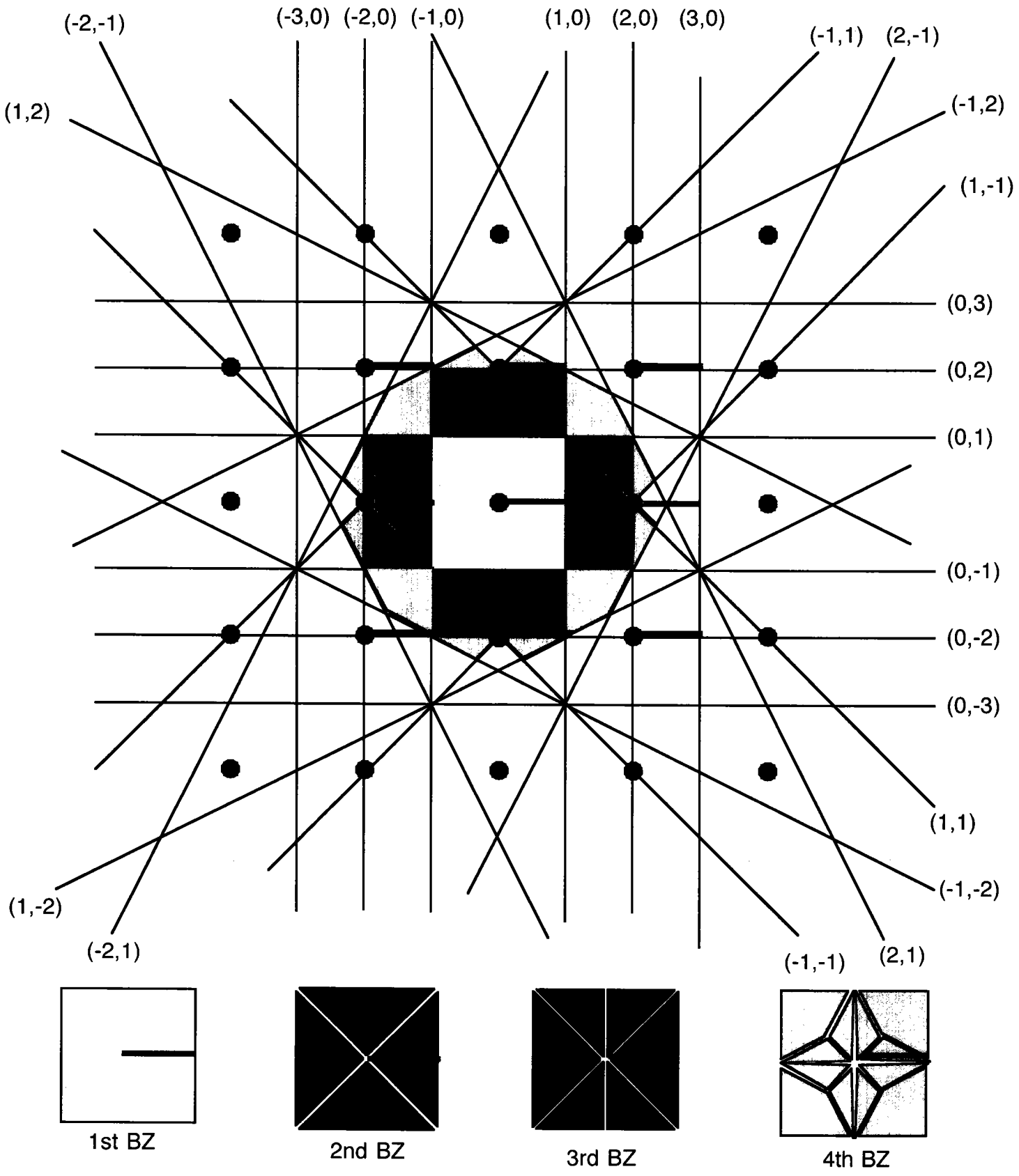
for $\vec{k} = k\hat{x}$ in 1st BZ, ie $0 < k < \frac{K}{2}$, we will plot the band structure, in reduced zone scheme, for all bands corresponding to the above set of R.L. vectors.

$$\varepsilon_i(\vec{k}) = \frac{\hbar^2}{2m}(\vec{k} - \vec{K}_i)^2$$

measure energy in units of $\varepsilon_x \equiv \frac{\hbar^2}{2m}\left(\frac{K}{2}\right)^2 = \frac{\hbar^2 K^2}{8m}$

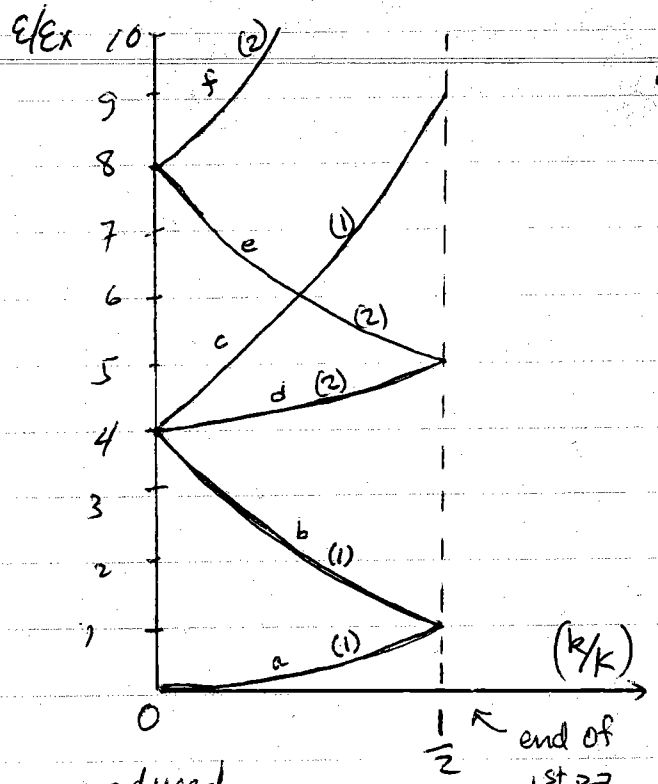
R.L. vector	energy	$\varepsilon/\varepsilon_x$	degeneracy	
$\vec{K}_0$:	$\varepsilon = \frac{\hbar^2}{2m}k^2$	$4(k/K)^2$	(1)	(a
$\{\vec{K}_1\}$: $+K\hat{x}$:	$\varepsilon = \frac{\hbar^2}{2m}(k-K)^2$	$4\left(\left(\frac{k}{K}\right)-1\right)^2$	(1)	(b
$\{\vec{K}_1\}$: $-K\hat{x}$:	$\varepsilon = \frac{\hbar^2}{2m}(k+K)^2$	$4\left(\left(\frac{k}{K}\right)+1\right)^2$	(1)	(c
$\{\vec{K}_1\}$: $\pm K\hat{y}$:	$\varepsilon = \frac{\hbar^2}{2m}(k^2+K^2)$	$4\left(\left(\frac{k}{K}\right)^2+1\right)$	(2)	(d
$\{\vec{K}_2\}$: $K(\hat{x}\pm\hat{y})$:	$\varepsilon = \frac{\hbar^2}{2m}\left[(k-K)^2+K^2\right]$	$4\left[\left(\frac{k}{K}-1\right)^2+1\right]$	(2)	(e
$\{\vec{K}_2\}$: $K(-\hat{x}\pm\hat{y})$:	$\varepsilon = \frac{\hbar^2}{2m}\left[(k+K)^2+K^2\right]$	$4\left[\left(\frac{k}{K}+1\right)^2+1\right]$	(2)	(f

Reciprocal Lattice and k-space for a two-dimensional square Bravais Lattice of lattice constant *a*.
Bragg planes are labeled by the reciprocal lattice vector that they bisect, $\mathbf{K} = (2\pi/a)(n, m)$.



Pieces of the nth Brillouin Zone translated back into the 1st BZ

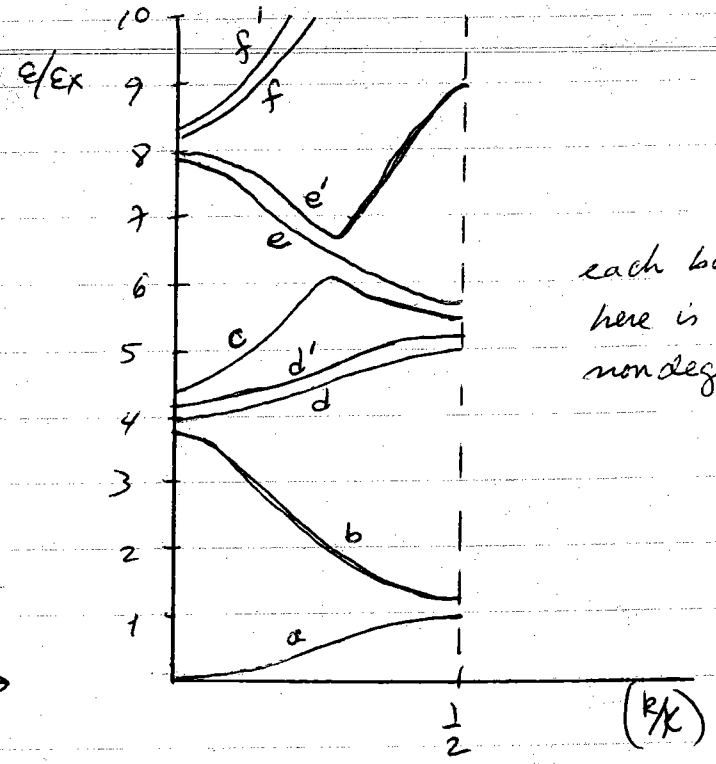
free electrons



reduced zone scheme

← end of 1st BZ in x̂ direction

weak potential



each band here is non degenerate

a) 1st BZ

b) 2nd BZ

d) 3rd + 4th BZs

c) 5th + 7th BZs

e) 5th, 6th + 7th BZs

f) 8th + 9th BZ + higher

a) 1st BZ

b) 2nd BZ

d) 3rd BZ

d') 4th BZ

c) 5th BZ

e) 6th BZ

e') 7th BZ

f) 8th BZ

f') 9th BZ

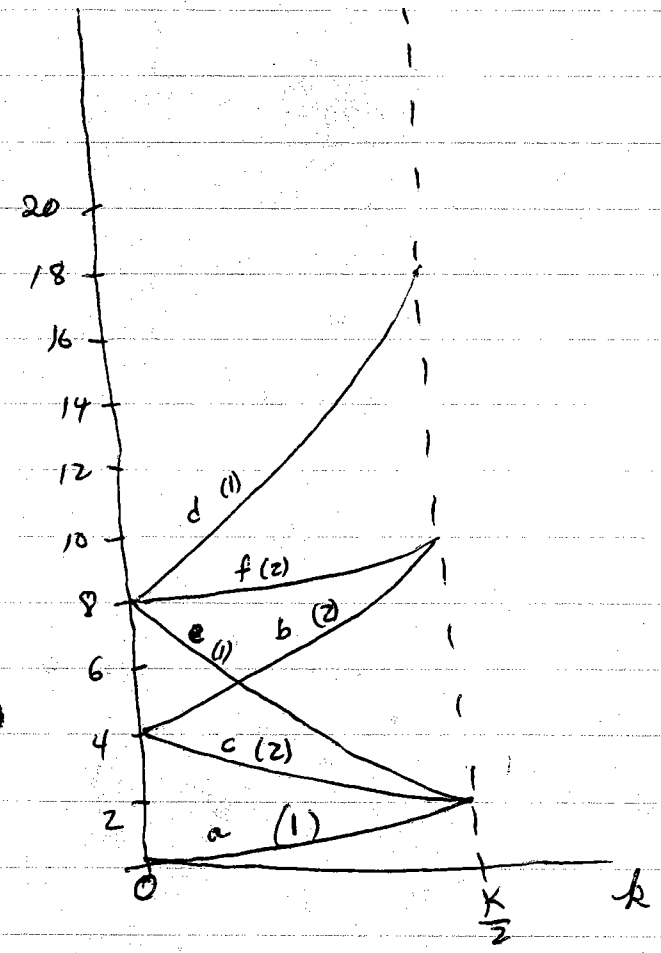
Weak potential splits degeneracies

More complicated band structure than in 1 dimension

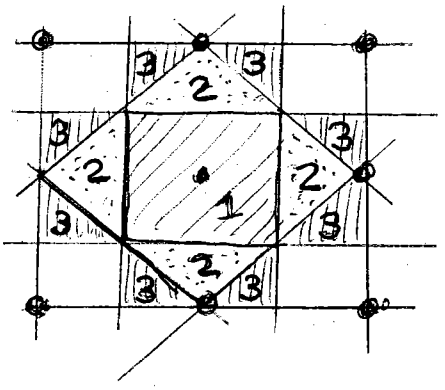
Not necessarily true that $\max\left[\mathcal{E}_n(\vec{k})\right] \leq \min\left[\mathcal{E}_{n+1}(\vec{k})\right]$

for $\vec{k} = k(\hat{x}+\hat{y})$ $\quad 0 < k < \frac{K}{2}$

R.L.	energy		degeneracy		
$\vec{K}_0$	$\varepsilon = \frac{\hbar^2 k^2}{2m}$ (2)	$\varepsilon/\varepsilon_x =$	$8\,(k/K)^2$	(1)	(a
$\{\vec{K}_1\}$ $-K\hat{x}, -K\hat{y}$	$\varepsilon = \frac{\hbar^2}{2m}\left[(k+K)^2 + k^2\right]$	$\varepsilon/\varepsilon_x = 4\left[\left(\frac{k}{K}+1\right)^2 + \left(\frac{k}{K}\right)^2\right]$		(2)	(b
$+K\hat{x}, +K\hat{y}$	$\varepsilon = \frac{\hbar^2}{2m}\left[(k-K)^2 + k^2\right]$	$\varepsilon/\varepsilon_x = 4\left[\left(\frac{k}{K}-1\right)^2 + \left(\frac{k}{K}\right)^2\right]$		(2)	(c
$\{\vec{K}_2\}$ $K(-\hat{x}-\hat{y})$	$\varepsilon = \frac{\hbar^2}{2m}\left[2(k+K)^2\right]$	$\varepsilon/\varepsilon_x = 8\left[\frac{k}{K}+1\right]^2$		(1)	(d
$K(+\hat{x}+\hat{y})$	$\varepsilon = \frac{\hbar^2}{2m}\left[2(k-K)^2\right]$	$\varepsilon/\varepsilon_x = 8\left[\frac{k}{K}-1\right]^2$		(1)	(e
$K(-\hat{x}+\hat{y})$ $K(\hat{x}-\hat{y})$	$\varepsilon = \frac{\hbar^2}{2m}\left[(k+K)^2 + (k-K)^2\right]$	$\varepsilon/\varepsilon_x = 4\left[\left(\frac{k}{K}+1\right)^2 + \left(\frac{k}{K}-1\right)^2\right]$		(2)	(f

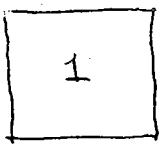


Zones in Two dimensions

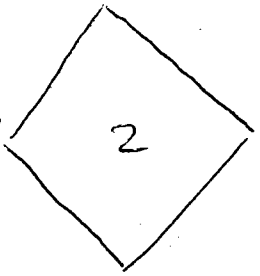


Draw in Bragg planes

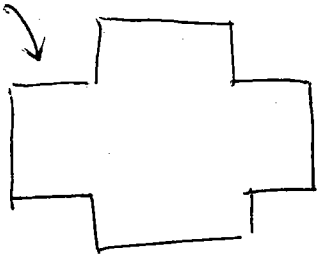
so outer surface 1st zone looks like



outer surface 2nd zone is →



outer surface 3rd zone is →



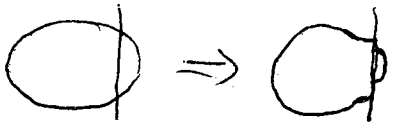
surface of nth zone gets more complicated as n increases

To find shape of constant energy surface (fermi surface) in weak potential approx:

1) Draw free fermi sphere corresponding to desired energy

2) See ~~which~~ which zones surface of sphere intersects
There will be branches of surface in each ~~zone~~ band corresponding to the zones

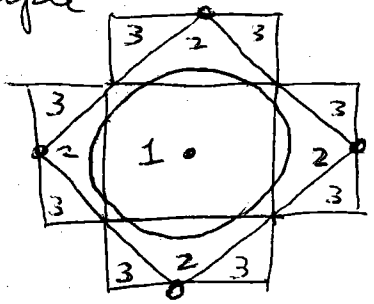
3) deform free energy sphere where it intersects zone boundary so that it is ⊥ to Bragg plane (HW prob #2)



(often ignore this step as 1st approx)

4) This gives constant energy surface in extended zone scheme. Translate branches of surface in nth zone back to 1st zone (by adding appropriate recip lattice vector) to get branches of surface in reduced zone scheme. Or translate through all recip lattice vectors to get repeated zone scheme.

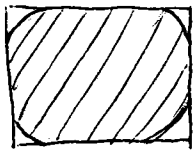
example



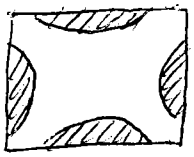
extended zone scheme

This free electron surface (of energy E_0) intersects 1st & 2nd zones only

Translate pieces of curves back to 1st BZ



branches of surface in 1st ~~zone~~ band.

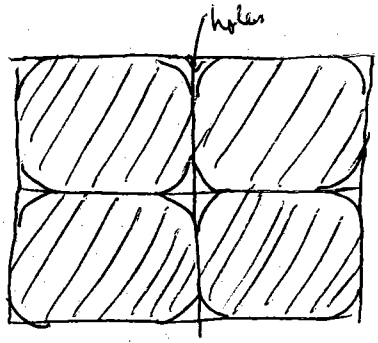


branches of surface in 2nd ~~zone~~ band translated back to 1st BZ

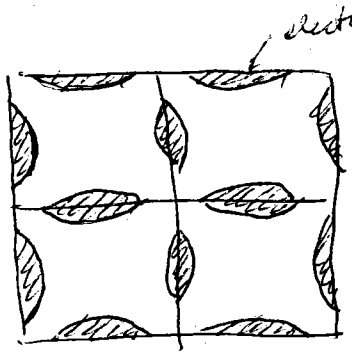
reduced zone scheme

Branches of curve in reduced zone scheme
Shaded areas are states of lower energy $\varepsilon < \varepsilon_0$.
Unshaded areas are states of greater energy $\varepsilon > \varepsilon_0$

In ~~extended~~ repeated zone scheme, branches look like



branches in 1st zone



branches in 2nd zone

branches of fermi surface are closed curves

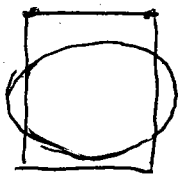
If surface we have drawn is Fermi surface, then shaded areas are filled states.

In 1st band we have small pockets of holes
In 2nd band we have small pockets of electrons

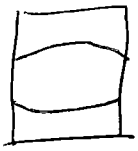
} more meaning to this when we get to dynamics

In both cases, the constant energy surface in the repeated zone scheme is a <u>closed</u> curve. This need not be the case for a less symmetric crystal

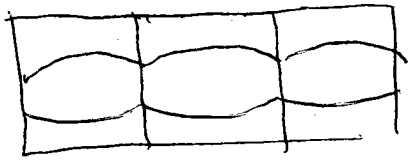
1st BZ



in this case, branches in 1st zone are



when we extend to repeated zone scheme we get



surface of constant energy is an <u>open</u> curve

The distinction between open and closed surfaces will be very important when we consider the dynamics (motion in magnetic field - energy conserved - electron moves on const energy surface)

See text for pictures in 3-D.

Note that in 2 + 3 dimensions, one always has partially full bands. ⇒ Weak potential method does not give insulators or semiconductors.

For pictures of Brillouin Zones, band structure, and Fermi surfaces in 3D, see text.