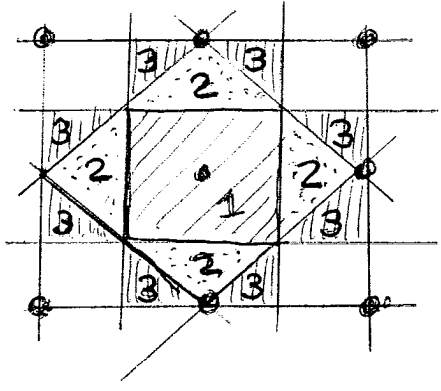


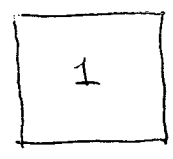
and Fermi Surface

Zones in Two dimensions - single square BL

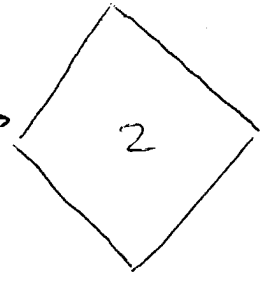
Draw in Bragg p planes



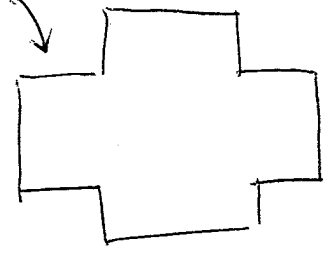
so ^{outer} surface 1st zone looks like



outer surface 2nd zone is →



outer surface 3rd zone is →

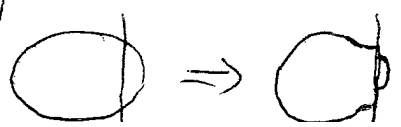


Surface of n th zone gets more complicated as n increases

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 ~~one~~ the} zones
- 3) deform free energy sphere where it intersects zone boundary so that it is \perp to Bragg plane (HW probl

#2)

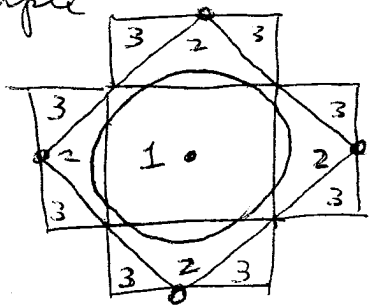


(often ignore this step as 1st approx)

4) This gives constant energy surface in extended zone scheme.
 Translate branches of surface in n th 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

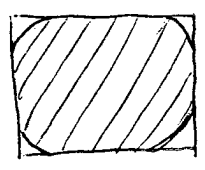
extended zone scheme



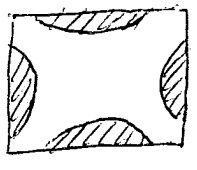
This free electron surface ^(of energy E_0) intersects 1st & 2nd zones only

Translate pieces of curves back to 1st BZ

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



reduced zone scheme



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

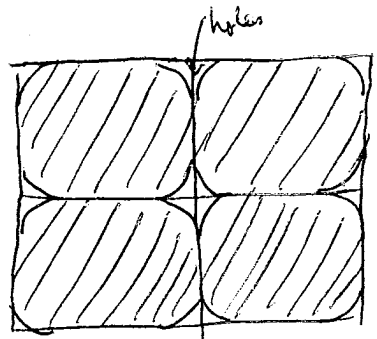
Branches of curve in reduced zone scheme

shaded areas are states of lower energy $E < E_0$.

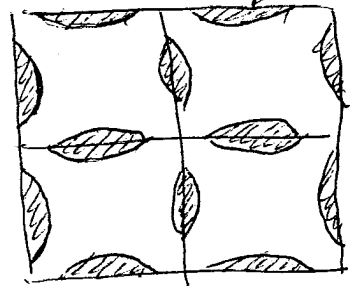
unshaded areas are states of greater energy $E > E_0$

In repeated zone scheme, branches look like

zones in 1st zone



cutouts



branches in 2nd zone

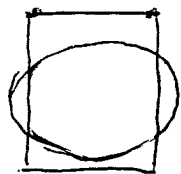
branches of Fermi surface are closed curves

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

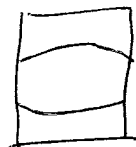
In 1st band we have small pockets of holes } more meaning
 In 2nd band we have small pockets of electrons } to this when
 we get to dynamics

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

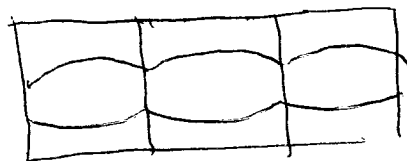
1st BZ



in this case, branches in 1st zone are



when we extend to repeated zone scheme we get



surface of constant energy is an open 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. \Rightarrow weak potential method does not give insulators or semiconductors.

See Ashcroft + Mermin Figs 9.8 and 9.9 for BZ's and Fermi surface branches in 3D

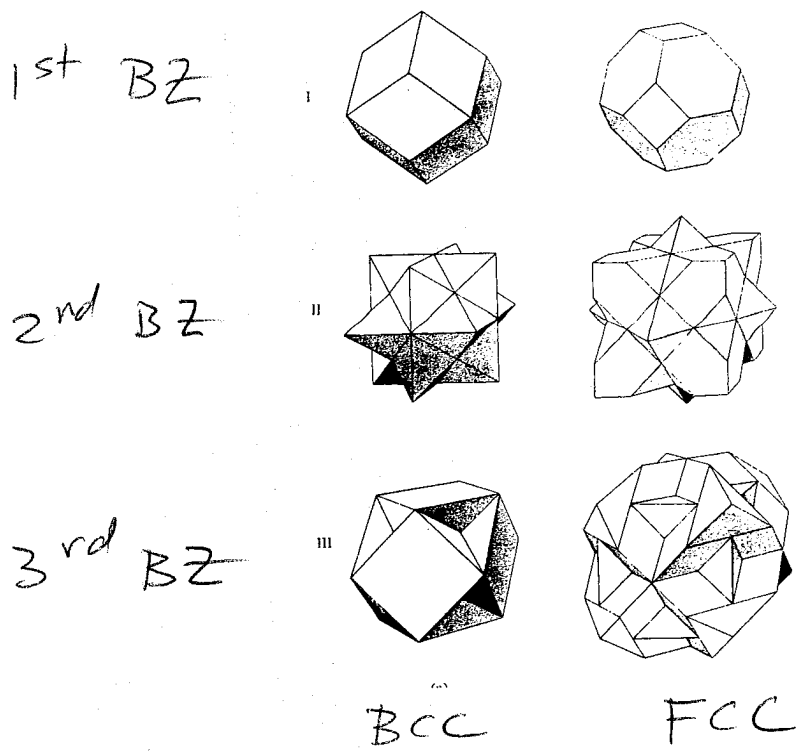


Figure 9.8 Surfaces of the first, second, and third Brillouin zones for (a) body-centered cubic and (b) face-centered cubic crystals. (Only the exterior surfaces are shown. It follows from the definition on page 163 that the interior surface of the n th zone is identical to the exterior surface of the $(n - 1)$ th zone.) Evidently the surfaces bounding the zones become increasingly complex as the zone number increases. In practice it is often simplest to construct free electron Fermi surfaces by procedures (such as those described in Problem 4) that avoid making use of the explicit form of the Brillouin zones. (After R. Lück, doctoral dissertation, Technische Hochschule, Stuttgart, 1965.)

Free electron Fermi surface FCC

$$Z = 4$$

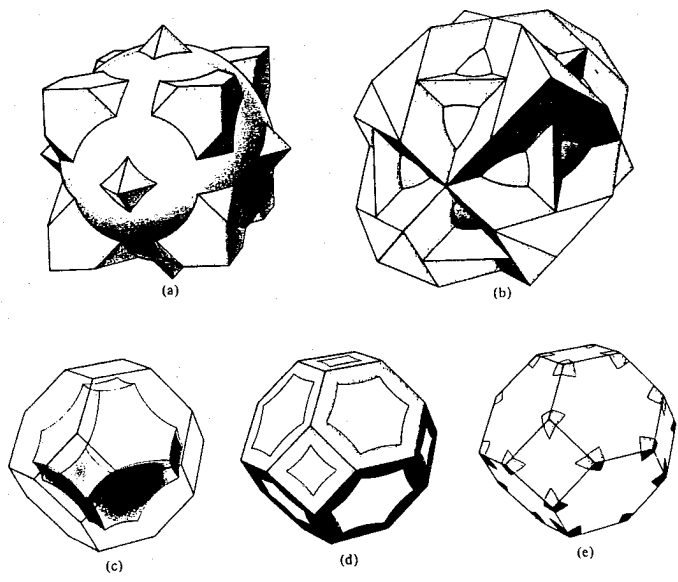
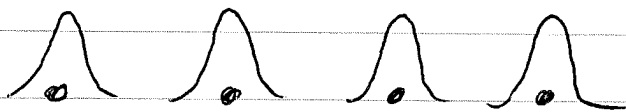


Figure 9.9 The free electron Fermi sphere for a face-centered cubic metal of valence 4. The first zone lies entirely within the interior of the sphere, and the sphere does not extend beyond the fourth zone. Thus the only zone surfaces intersected by the surface of the sphere are the (exterior) surfaces of the second and third zones (cf. Figure 9.8b). The second-zone Fermi surface consists of those parts of the surface of the sphere lying entirely within the polyhedron bounding the second zone (i.e., all of the sphere except the parts extending beyond the polyhedron in (a)). When translated through reciprocal lattice vectors into the first zone, the pieces of the second-zone surface give the simply connected figure shown in (c). (It is known as a "hole surface"; the levels it encloses have higher energies than those outside). The third-zone Fermi surface consists of those parts of the surface of the sphere lying outside of the second zone (i.e., the parts extending beyond the polyhedron in (a)) that do not lie outside the third zone (i.e., that are contained within the polyhedron shown in (b)). When translated through reciprocal lattice vectors into the first zone, these pieces of sphere give the multiply connected structure shown in (d). The fourth-zone Fermi surface consists of the remaining parts of the surface of the sphere that lie outside the third zone (as shown in (b)). When translated through reciprocal lattice vectors into the first zone they form the "pockets of electrons" shown in (e). For clarity (d) and (e) show only the intersection of the third and fourth zone Fermi surfaces with the surface of the first zone. (From R. Lück, *op. cit.*)

Tight Binding method

If ions are spaced far apart on the length scale on which the atomic bound state wavefunction decays, then expect that atomic wavefunctions will give a good approximation to the Bloch electron eigenstate in the periodic potential of all ions.



However the tails of the atomic wavefunctions will overlap allowing the electron to hop from ion to ion, behaving like a free Bloch electron.

For simplicity, assume the atomic valence electron is a single "s" ^{orbital} ~~shell~~ electron. This atomic state is non-degenerate. Let its wavefunction be $\phi_0(\vec{r})$ for ion centered at origin.

We can construct a Bloch electron state out of the individual atomic states $\phi_0(\vec{r}-\vec{R}_i)$ by

$$\psi_{\vec{k}}(\vec{r}) = \sum_i e^{i\vec{k} \cdot \vec{R}_i} \phi_0(\vec{r}-\vec{R}_i)$$

Counting: We go from N atomic wavefunctions $\phi_0(\vec{r}-\vec{R}_i)$, N values of \vec{R}_i , to N Bloch wavefunctions $\psi_{\vec{k}}(\vec{r})$, N values of \vec{k} in 1st BZ.

(only mix atomic wavefunctions $\phi_0(\vec{r}-\vec{R}_i)$ where electron has same spin value)

$$\text{Let } H = H_{\text{at}} + \Delta U$$

H is Hamiltonian of entire system

H_{at} is Hamiltonian of atom at origin

ΔU is potential from all atoms except the one at the origin

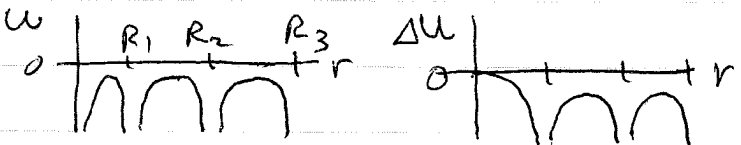
i.e. if total potential is $U(\vec{r}) = \sum_{\vec{R}_i} v(\vec{r} - \vec{R}_i)$
 \vec{R}_i \uparrow atomic potential

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

$$H_{\text{at}} = \frac{p^2}{2m} + v(\vec{r})$$

$$\Delta U = \sum_{\vec{R}_i \neq 0} v(\vec{r} - \vec{R}_i) = U(\vec{r}) - v(\vec{r})$$

choose energy scale so that $\Delta U(0) = 0$,

Now consider: 

$$\langle \psi_0 | H | \psi_k \rangle = \langle \psi_0 | H_{\text{at}} + \Delta U | \psi_k \rangle$$

$$E_k \langle \psi_0 | \psi_k \rangle = E_a \langle \psi_0 | \psi_k \rangle + \langle \psi_0 | \Delta U | \psi_k \rangle$$

\uparrow

energy of Bloch state ψ_k

\uparrow

atomic energy level of ψ_0

$$E_k = E_a + \frac{\langle \psi_0 | \Delta U | \psi_k \rangle}{\langle \psi_0 | \psi_k \rangle}$$

$$\begin{aligned}
 \langle \psi_0 | \psi_k \rangle &= \sum_i e^{i\vec{k} \cdot \vec{R}_i} \int d^3r \psi_0^*(\vec{r}) \psi_0(\vec{r} - \vec{R}_i) \\
 &= 1 + \sum_{\substack{R_i \neq 0 \\ \uparrow \\ \text{from } \vec{R}_i = 0}} e^{i\vec{k} \cdot \vec{R}_i} \underbrace{\int d^3r \psi_0^*(\vec{r}) \psi_0(\vec{r} - \vec{R}_i)}_{\text{overlap}}
 \end{aligned}$$

If cons are far apart, overlap integrals are small. Only keep nearest neighbor terms, i.e. only sum over the smallest non-zero values of \vec{R}_i .

$$\langle \psi_0 | \psi_k \rangle = 1 + \sum_{nn} e^{i\vec{k} \cdot \vec{R}_i} \underbrace{\int d^3r \psi_0^*(\vec{r}) \psi_0(\vec{r} - \vec{R}_i)}_{\propto \alpha(\vec{R}_i)}$$

$$\langle \psi_0 | \psi_k \rangle = 1 + \sum_{nn} e^{i\vec{k} \cdot \vec{R}_i} \alpha(\vec{R}_i) \quad \alpha \text{ is small}$$

$$\begin{aligned}
 \langle \psi_0 | \Delta U | \psi_k \rangle &= \sum_i e^{i\vec{k} \cdot \vec{R}_i} \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r} - \vec{R}_i) \\
 &= \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r}) \\
 &\quad + \sum_{\substack{R_i \neq 0 \\ \uparrow \\ \text{from } \vec{R}_i = 0}} e^{i\vec{k} \cdot \vec{R}_i} \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r} - \vec{R}_i)
 \end{aligned}$$

again, keep only terms for nearest neighbor \vec{R}_i .

$$\text{define } \beta \equiv - \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r})$$

$$\gamma(\vec{R}) \equiv - \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r} - \vec{R}_i)$$

$$\langle \psi_0 | \Delta U | \psi_k \rangle = -\beta - \sum_{nn} e^{i\vec{k} \cdot \vec{R}_i} \gamma(\vec{R}_i)$$

$$E_k = E_a - \left[\frac{\beta + \sum_{nn} e^{i\vec{k}\cdot\vec{R}_i} \gamma(\vec{R})}{1 + \sum_{nn} e^{i\vec{k}\cdot\vec{R}_i} \alpha(\vec{R})} \right]$$

$$E_k \approx E_a - \beta - \sum_{nn} e^{i\vec{k}\cdot\vec{R}_i} (\gamma(\vec{R}) - \beta\alpha(\vec{R}))$$

since α small, $\frac{1}{1+\alpha} \approx 1-\alpha$

New $\alpha(\vec{R}) = \int d^3r \psi_0^*(\vec{r}) \psi_0(\vec{r}-\vec{R}) = \int d^3r \psi_0^*(\vec{r}+\vec{R}) \psi_0(\vec{r})$
 $= \alpha^*(-\vec{R})$

For s-orbital has real wave function $\psi_0 \Rightarrow \alpha = \alpha^*$
 so $\alpha(\vec{R}) = \alpha(-\vec{R})$

$$\begin{aligned} \gamma(\vec{R}) &= - \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r}-\vec{R}) && \text{take } \vec{r} \rightarrow -\vec{r} \\ &= - \int d^3r \psi_0^*(-\vec{r}) \Delta U(-\vec{r}) \psi_0(-\vec{r}-\vec{R}) \end{aligned}$$

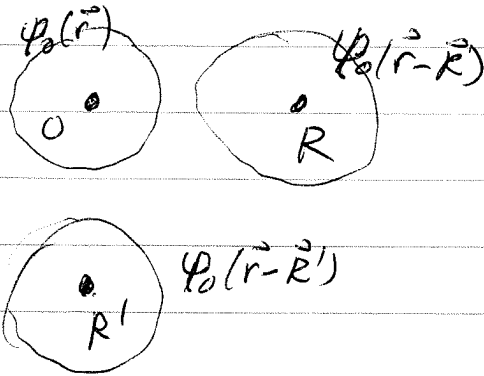
If crystal has inversion symmetry, i.e. $\Delta U(-\vec{r}) = \Delta U(\vec{r})$
 and since s-orbital is spherically symmetric, i.e. $\psi_0(\vec{r})$ depends only on $|\vec{r}|$ so $\psi_0(\vec{r}) = \psi_0(-\vec{r})$, then

$$= - \int d^3r \psi_0^*(\vec{r}) \Delta U(\vec{r}) \psi_0(\vec{r}+\vec{R}) = \gamma(-\vec{R})$$

so $\gamma(\vec{R}) = \gamma(-\vec{R})$ and $\alpha(\vec{R}) = \alpha(-\vec{R})$

$$E_k = E_a - \beta - \sum_{nn} [\gamma(\vec{R}) - \beta\alpha(\vec{R})] \cos \vec{k}\cdot\vec{R}$$

Moreover if the crystal has cubic symmetry, then since ψ_0 is rotationally symmetric, $\gamma(\vec{R})$ and $\alpha(\vec{R})$ will be the same value for all n in \vec{R}



All will have cubic symmetry so $\gamma(\vec{R}) = \gamma(\vec{R}')$
 $\alpha(\vec{R}) = \alpha(\vec{R}')$

$$E_k = E_a - \beta - \tilde{\gamma} \sum_{nn} \cos(\vec{k} \cdot \vec{R}) \quad \tilde{\gamma} = \gamma - \beta\alpha$$

See A+M for case of fcc lattice.

Here we consider the simpler sc lattice

$$n \vec{R} \text{ are } \pm a \hat{x}, \pm a \hat{y}, \pm a \hat{z}$$

$$\vec{R} \cdot \vec{R} \text{ are } \pm k_x a, \pm k_y a, \pm k_z a$$

$$E_k = E_a - \beta - 2\tilde{\gamma} (\cos k_x a + \cos k_y a + \cos k_z a)$$

band width $E_k^{\max} - E_k^{\min} = 12\tilde{\gamma}$

for small k , $\cos ka \approx 1 - \frac{1}{2} k^2 a^2$

$$E_k \approx E_a - \beta - 2\tilde{\gamma} \left(3 - \frac{1}{2} k_x^2 a^2 - \frac{1}{2} k_y^2 a^2 - \frac{1}{2} k_z^2 a^2 \right)$$

$$\approx E_a - \beta - 6\tilde{\gamma} + \tilde{\gamma} k^2 a^2$$