Fermi surfaces and metals

- Higher BZ, Fermi surface
- Semiclassical electron dynamics (see Chap 8)
- de Haas-van Alphen effect

(the Sec on "Calculation of energy bands" will be skipped)

Dept of Phys

M.C. Chang

First,

- A filled band does not carry current (Peierls, 1929)

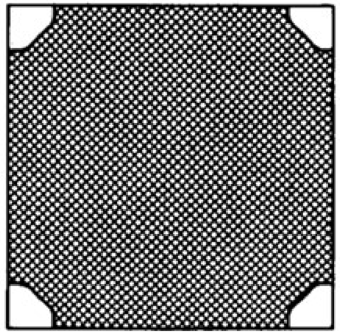
- The concept of hole

A nearly-filled band

$$\vec{j} = -\frac{e}{V}\sum_{\text{filled }\vec{k}} \vec{v}$$

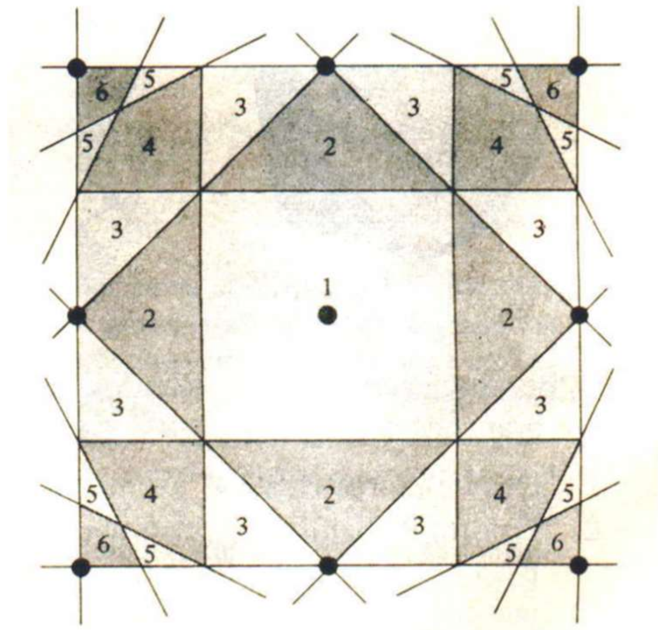
$$= -\frac{e}{V}\left(\sum_{\vec{k}\in \text{1st BZ}} \vec{v} - \sum_{\text{unfilled }\vec{k}} \vec{v} \right)$$

$$= +\frac{e}{V}\sum_{\text{unfilled }\vec{k}} \vec{v}$$

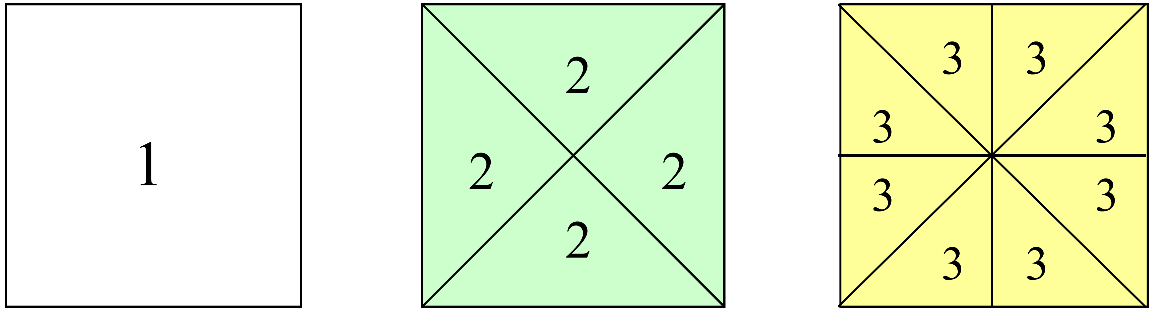


$\therefore$ unoccupied states behave as +e charge carriers

• Beyond 1st Brillouin zone
(for square lattice)



• Reduced zone scheme

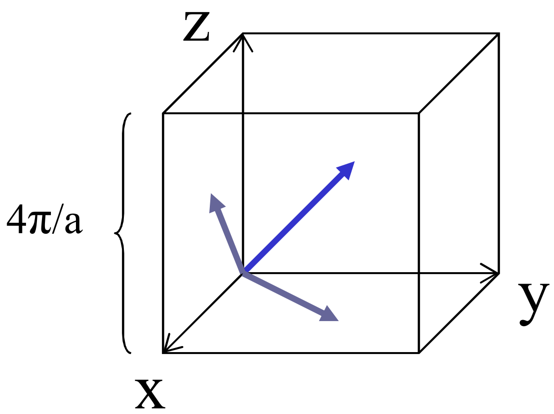


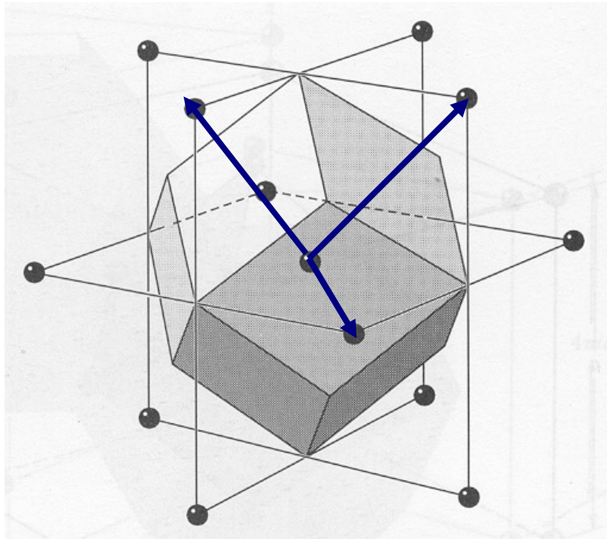
Every Brillouin zone has the same area

• At zone boundary, **k** satisfies the Laue condition $\vec{k} \cdot \hat{G} = \dfrac{G}{2}$

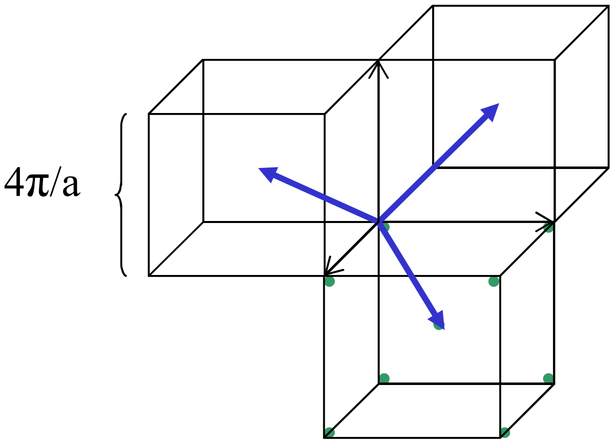
Bragg reflection at zone boundaries produce energy gaps

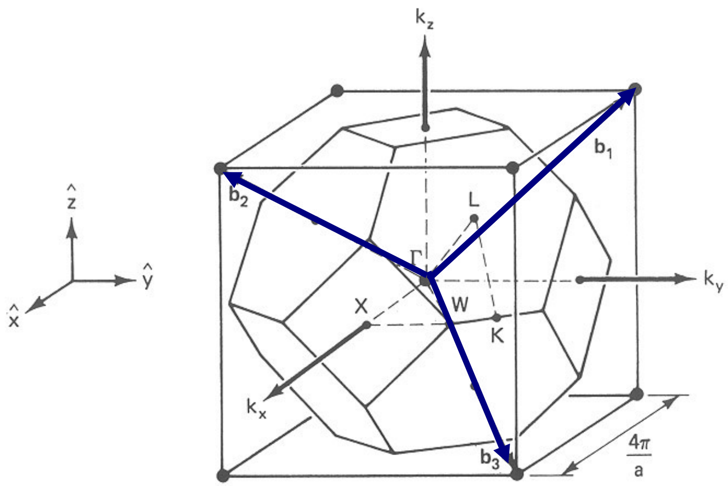
- The first BZ of bcc lattice (its reciprocal lattice is fcc lattice)





- The first BZ of fcc lattice (its reciprocal lattice is bcc lattice)

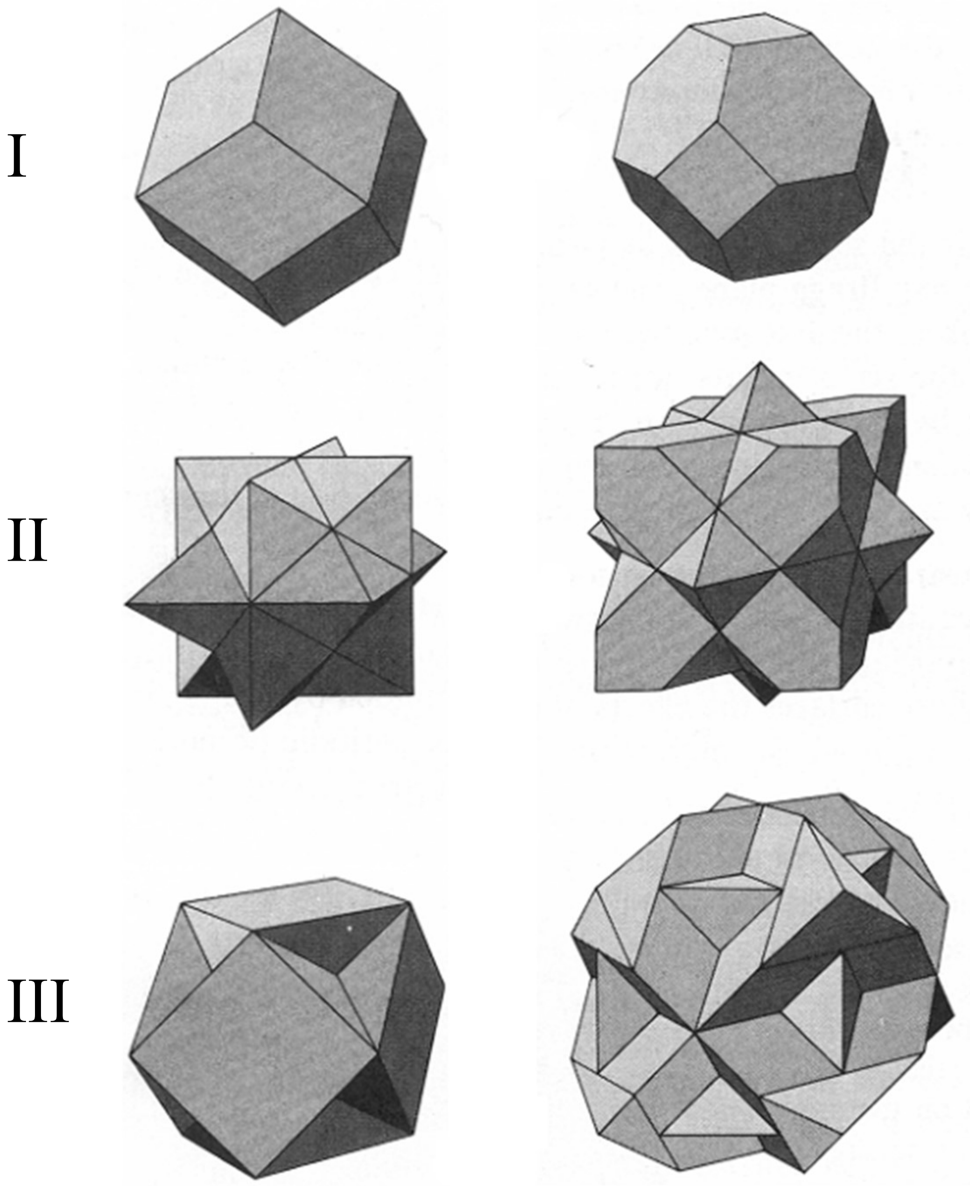




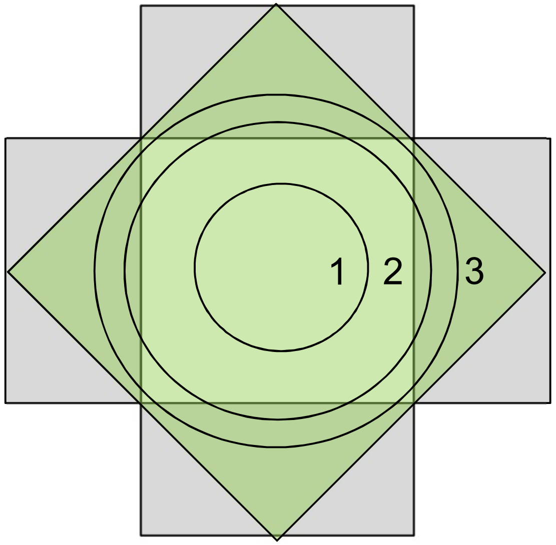
Beyond the 1st Brillouin zone

BCC crystal
(e.g. Alkali metal)

FCC crystal
(e.g. noble metal)



Fermi surface for 2D *empty* square lattice



- For a *monovalent* element, the Fermi wave vector

$$k_F = \sqrt{2\pi}/a$$

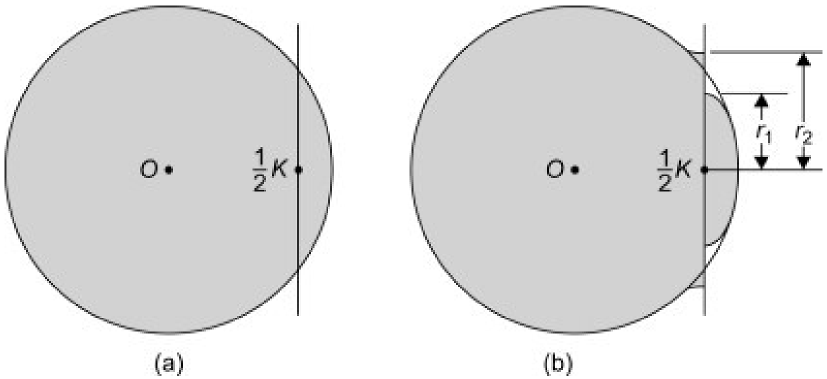
- For a *divalent* element

$$k_F = \sqrt{4\pi}/a$$

- For a *trivalent* element

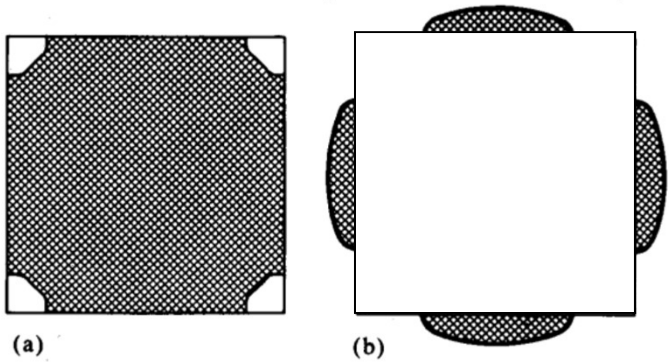
$$k_F = \sqrt{6\pi}/a$$

- Distortion due to lattice potential



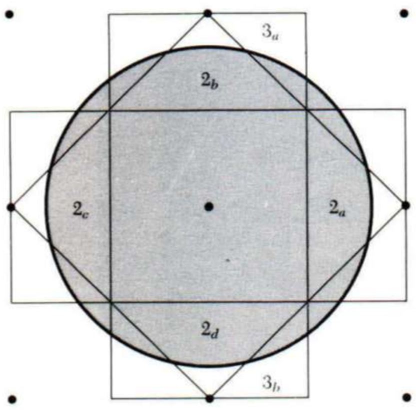
Chap 9 of A+M, Prob.1 $r_2^2 - r_1^2 \propto |U_{\vec{G}}|$

1st BZ 2nd BZ

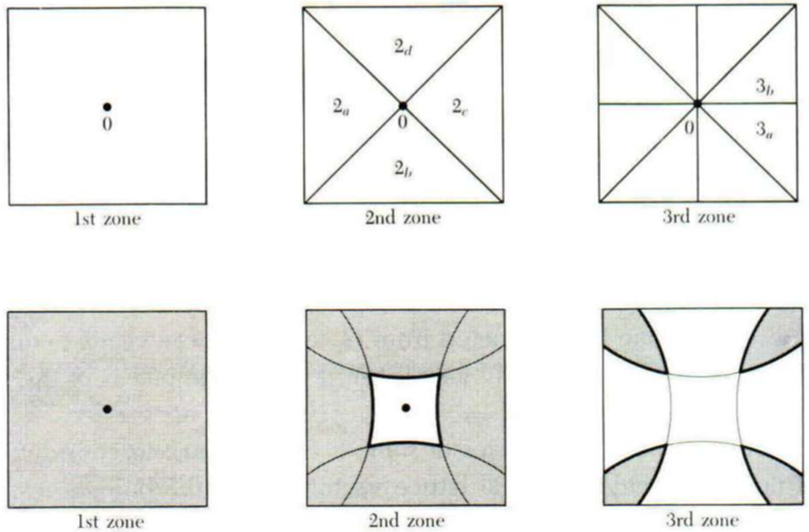


A larger Fermi sphere (empty lattice)

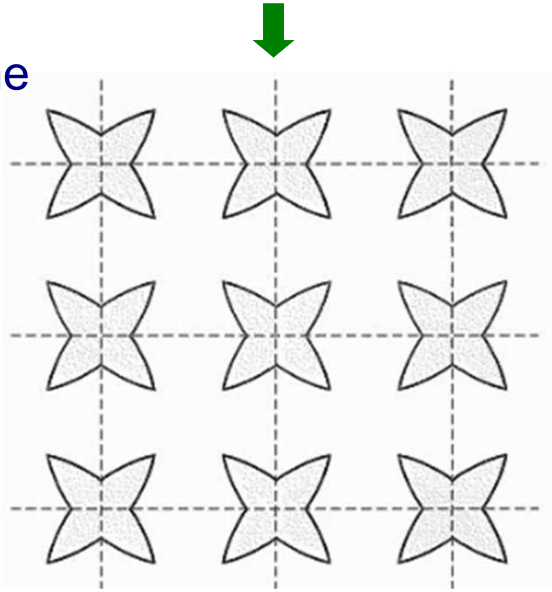
- Extended zone scheme



- Reduced zone scheme



- Periodic zone scheme



Again if we turn on the lattice potential, then the corners become rounded.

Fermi surface of alkali metal (monovalent, BCC)

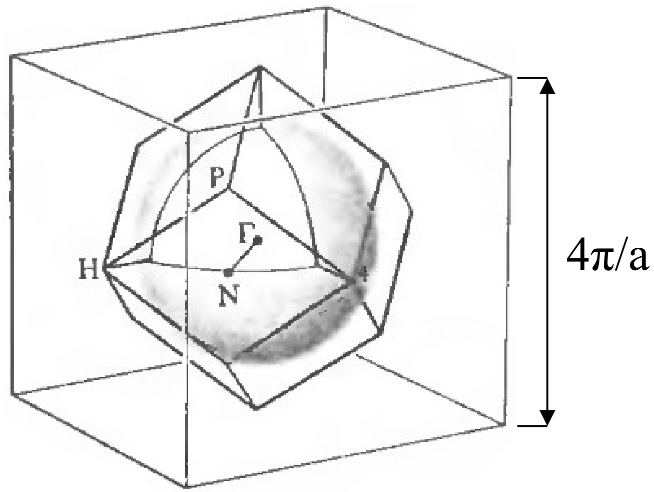
$k_F = (3\pi^2 n)^{1/3}$

$n = 2/a^3$

$\rightarrow k_F = (3/4\pi)^{1/3}(2\pi/a)$

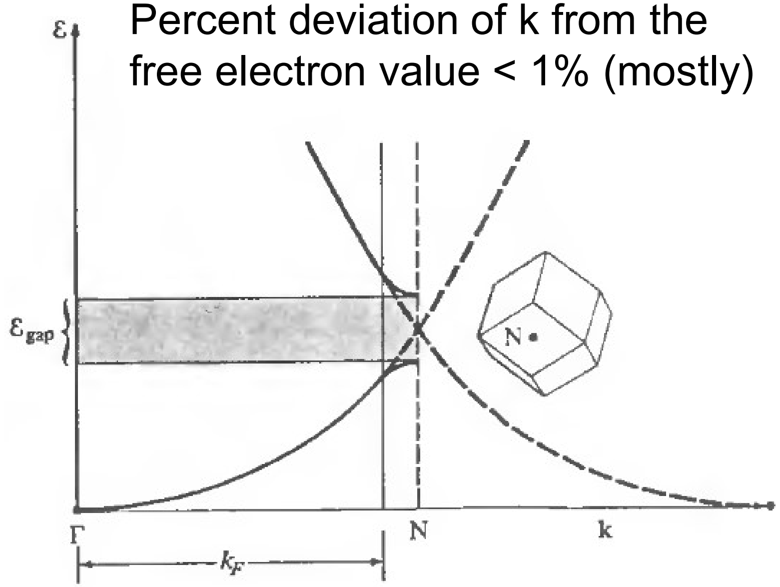
$\Gamma N = (2\pi/a)[1/2]^{1/2}$

$\therefore k_F = 0.877\ \Gamma N$



1st Brillouin zone

Percent deviation of k from the free electron value < 1% (mostly)



THE MONOVALENT METALS

ALKALI METALS (BODY-CENTERED CUBIC)[a]		NOBLE METALS (FACE-CENTERED CUBIC)	
Li:	$1s^2 2s^1$	—	
Na:	$[Ne]3s^1$	—	
K:	$[Ar]4s^1$	Cu:	$[Ar]3d^{10}4s^1$
Rb:	$[Kr]5s^1$	Ag:	$[Kr]4d^{10}5s^1$
Cs:	$[Xe]6s^1$	Au:	$[Xe]4f^{14}5d^{10}6s^1$

Fermi surface of noble metal (monovalent, FCC)

$k_F = (3\pi^2 n)^{1/3}$,

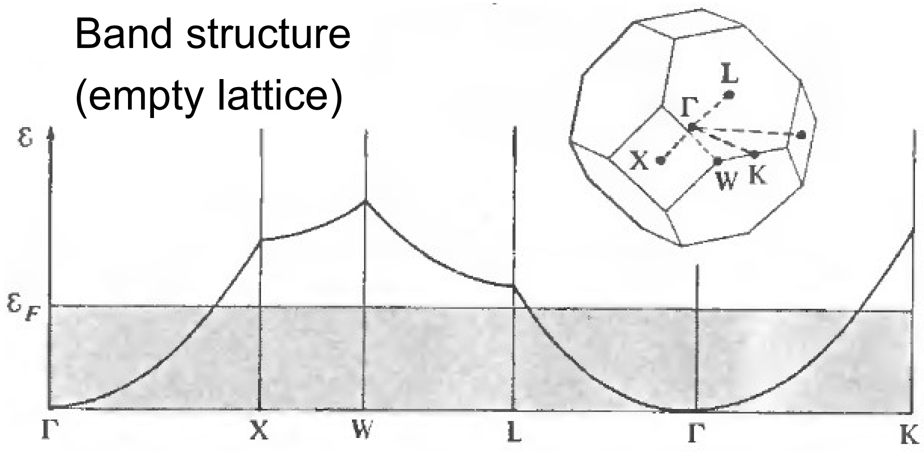
$n = 4/a^3$

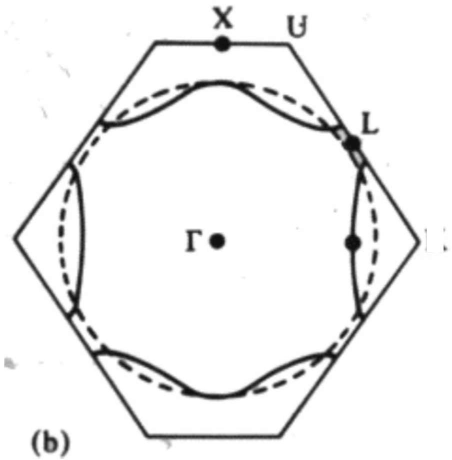
$\rightarrow k_F = (3/2\pi)^{1/3}(2\pi/a)$

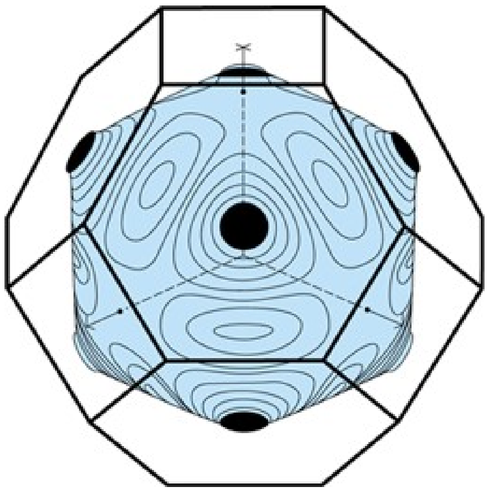
$\Gamma L =$ ___

$k_F =$ ___ ΓL

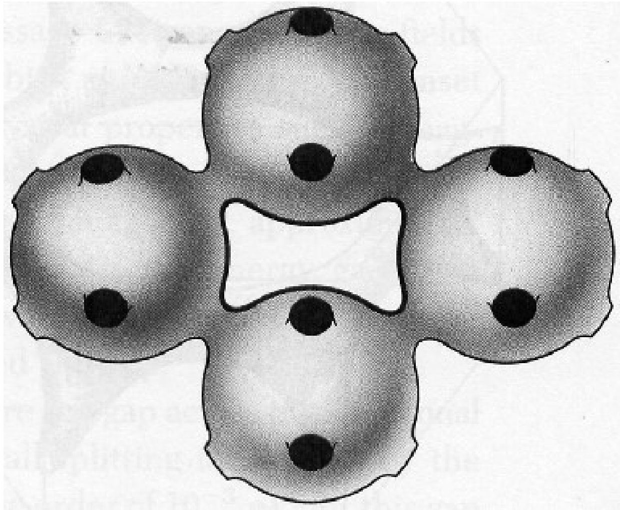
Band structure
(empty lattice)





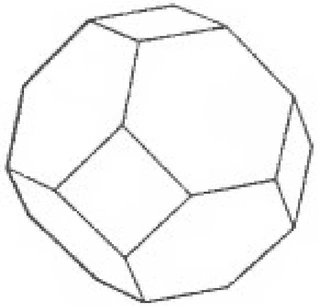


Periodic zone scheme

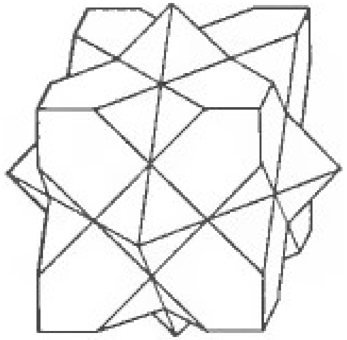


Fermi surface of Al (trivalent, FCC)

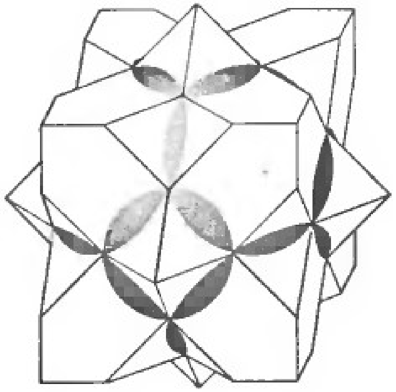
1st BZ



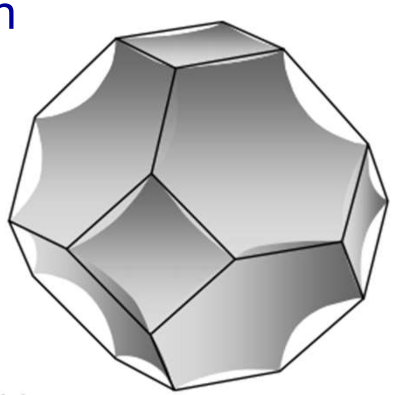
2nd BZ



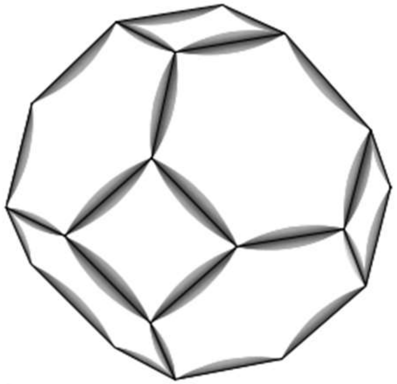
- Empty lattice approximation



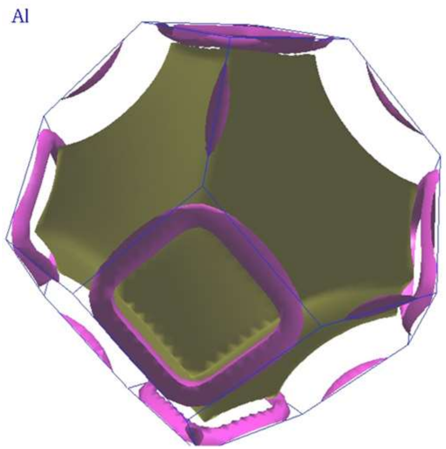
2nd BZ



3rd BZ

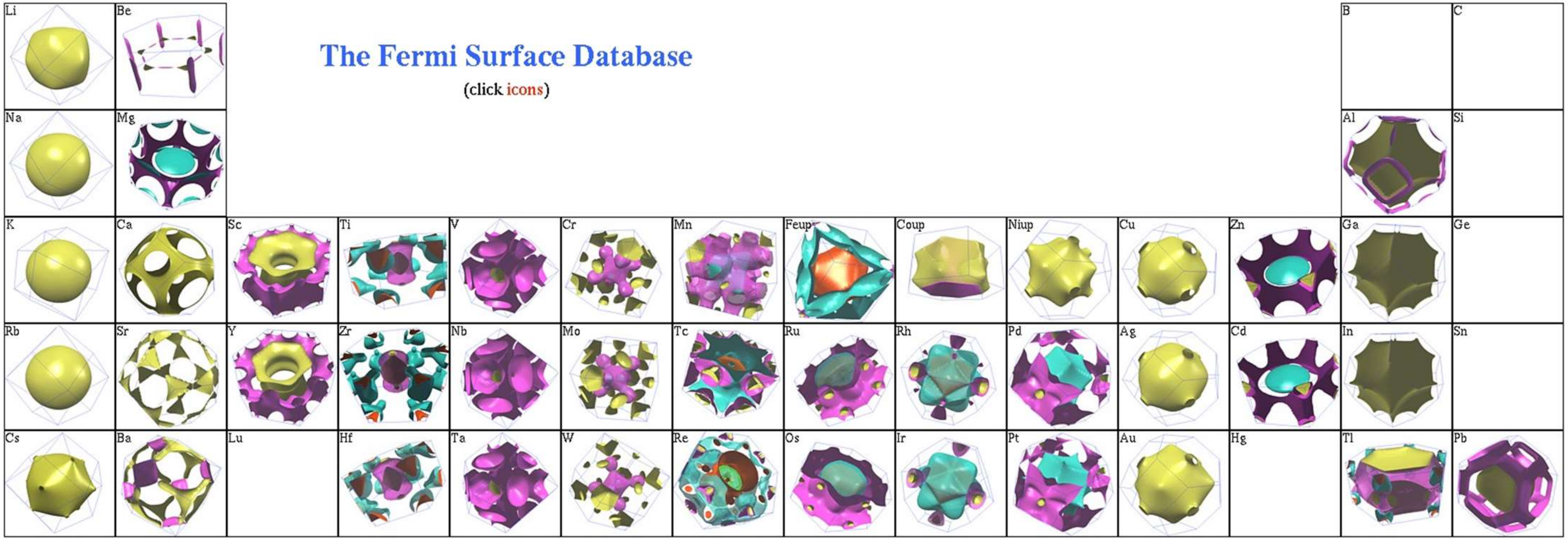


- Actual Fermi surface



Ref: Fermi surface database

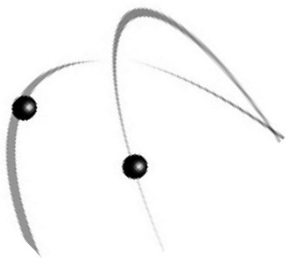
www.phys.ufl.edu/fermisurface/



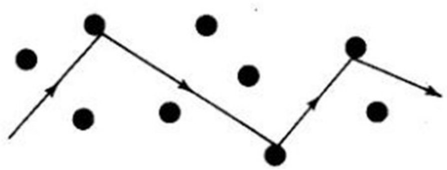
- Higher BZ, Fermi surface
- Semiclassical electron dynamics
- de Haas-van Alphen effect

In what follows, CGS is used.
To convert to SI, just set c=1.

Classical picture
(Drude, Lorentz)
Particle (localized)



Electron scattering



Quantum picture
(Sommerfeld, Bloch)
Bloch wave (extended)

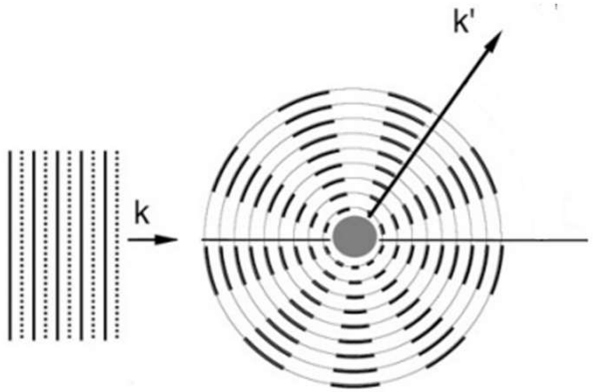
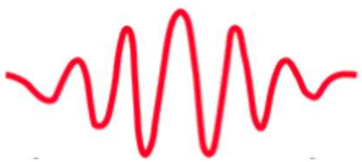


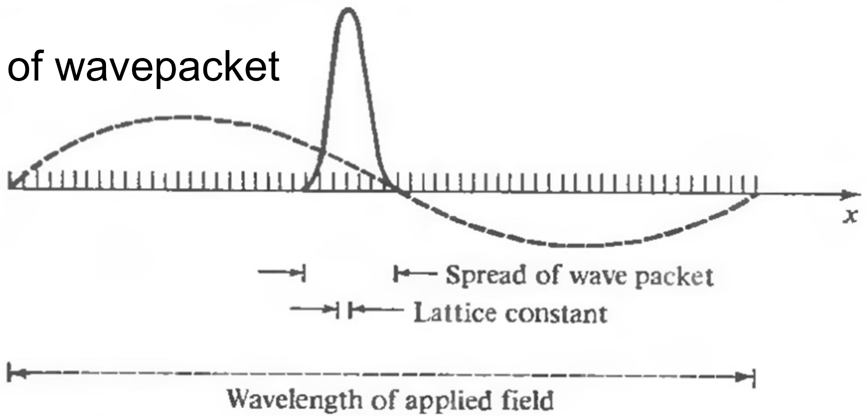
Fig from Simons Lab

Semiclassical picture
- Wavepacket



(Superposition of Bloch states)

Scale of wavepacket



important

Semiclassical electron dynamics (Chap 8)

Equation of motion for a wave packet in band-*n* with location *r* and wavevector *k*:

$$\begin{cases} \dot{\vec{r}}(\vec{k}) = \dfrac{1}{\hbar}\dfrac{\partial \varepsilon_n(\vec{k})}{\partial \vec{k}} \\ \hbar\dot{\vec{k}} = q\left(\vec{E} + \dfrac{\dot{\vec{r}}(\vec{k})}{c}\times\vec{B}\right) \end{cases}$$

Derivation neglected

- ***E*** is the external field, not including the lattice field.

The effect of lattice is hidden in $\varepsilon_n(\boldsymbol{k})$!

Range of validity

- It is valid only when inter-band transition can be neglected.

"never close to being violated in a metal"

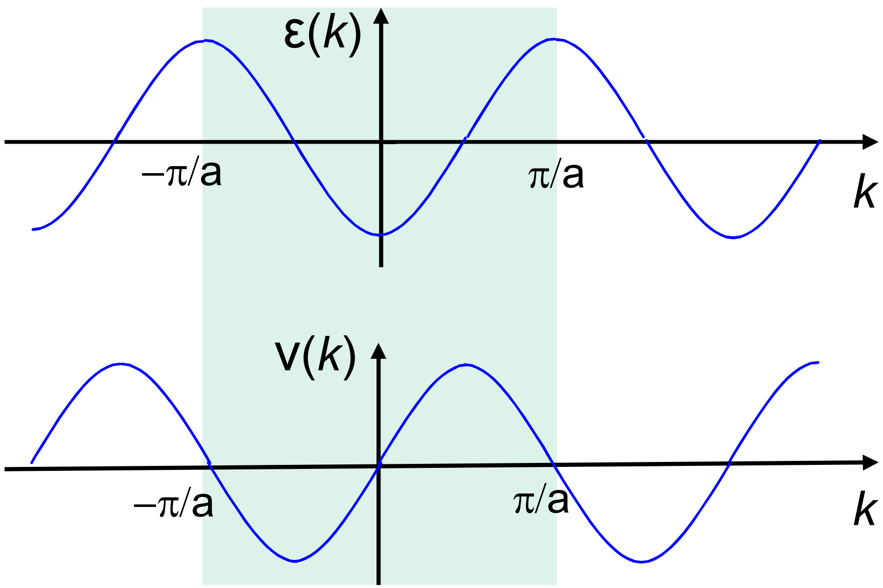
That is, the electron moves in one band only.

(One band approximation)

Bloch electron in an uniform electric field (Kittel, p.197)

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{E} \rightarrow \hbar\vec{k}(t) = -e\vec{E}t$$

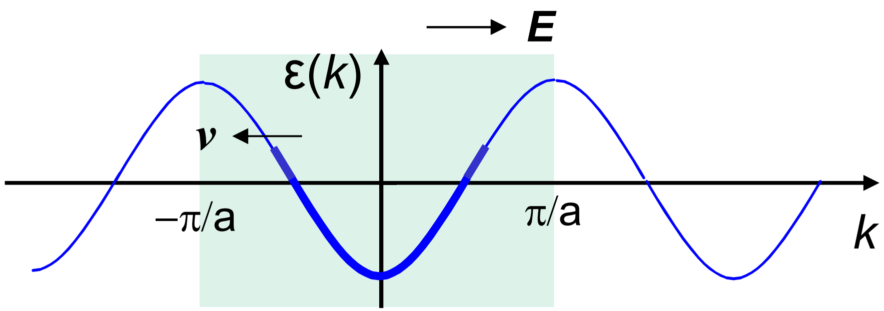
• Energy dispersion (1D, periodic zone scheme)



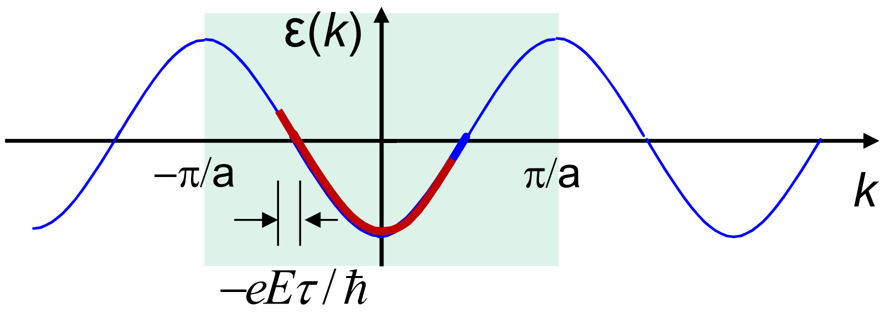
• In a DC electric field, the electrons decelerate and reverse its motion at the BZ boundary.

• A DC bias produces an AC current! (called Bloch oscillation)

- Partially filled band without scattering



- Partially filled band with scattering time τ



- Current density

$$j = (-e)\frac{1}{V}\sum_{k\,\in \text{filled states}} v_k$$

• Why the oscillation is not observed?

The electron has to maintain phase coherence.

To complete a cycle (*a* is the lattice constant),

$$eET/\hbar = 2\pi/a \rightarrow T = h/eEa$$

For $E=10^4$ V/cm, and $a=1$ A, $T=10^{-10}$ s.

But electron collisions take only about 10^{-14} s.

∴ a Bloch electron cannot reach zone boundary without de-phasing.

To observe it, one needs

- a stronger *E* field → but only up to about 10^6 V/cm (for semicond)
- a larger *a* → use superlattice (eg. a = 100 A)
- reduce collision time → use crystals with high quality

(Mendez et al, PRL, 1988)

• Bloch oscillators generate THz microwave:

frequency $\sim 10^{12\sim13}$,

wave length $\lambda \sim$ 0.01 mm - 0.1mm

(Waschke et al, PRL, 1993)

important

Bloch electron in an uniform magnetic field

$$\hbar \frac{d\vec{k}}{dt} = -e\frac{\vec{v}}{c}\times\vec{B}, \quad \vec{v}_k = \frac{1}{\hbar}\frac{\partial\varepsilon(\vec{k})}{\partial\vec{k}}$$

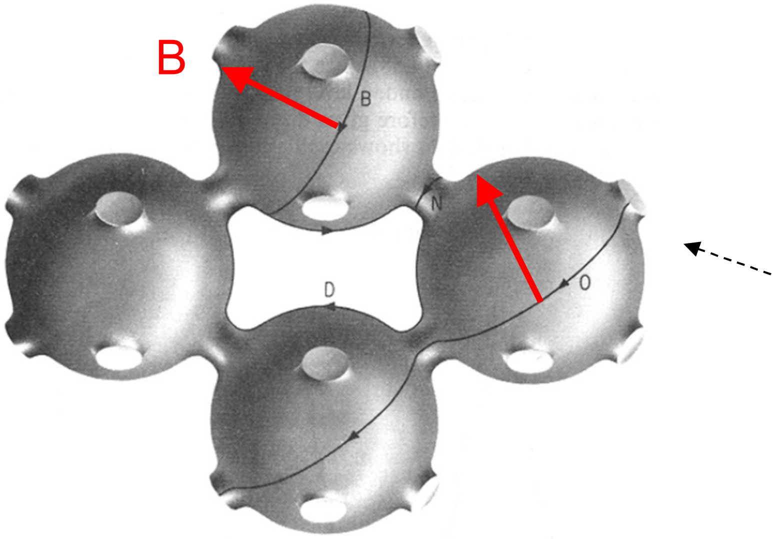
$$\rightarrow \dot{\vec{k}}\cdot\vec{B} = 0, \quad \dot{\vec{k}}\cdot\vec{v}_k = \frac{1}{\hbar}\frac{d\varepsilon(\vec{k})}{dt} = 0$$

Therefore, 1. Change of *k* is perpendicular to ***B***,

$k_{||}$ does not change

and 2. ε(*k*) is a constant of motion

This determines uniquely an orbit on the FS (given I.C.):



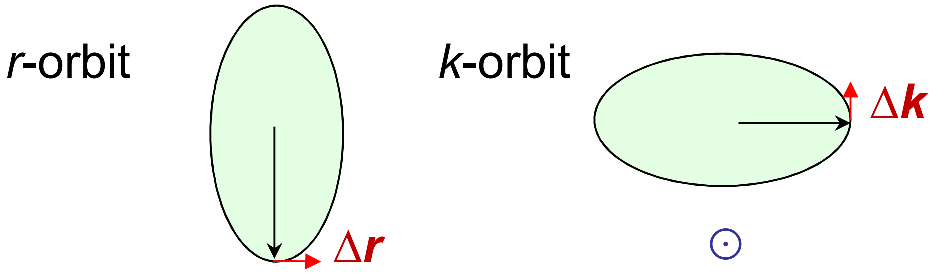
- For a *spherical* FS, it just gives the cyclotron orbit.
- For a connected FS, there might be open orbit.

Cyclotron orbit in real space

The analysis above gives us the orbit in *k*-space.
What about the orbit in *r*-space?

$$\hbar\dot{\vec{k}} = -\frac{e}{c}\dot{\vec{r}}\times\vec{B} \rightarrow \dot{\vec{r}} = -\frac{\hbar c}{eB^2}\vec{B}\times\dot{\vec{k}} + \dot{\vec{r}}_{\parallel}$$

$$\rightarrow \vec{r}_{\perp}(t) - \vec{r}_{\perp}(0) = -\frac{\hbar c}{eB}\hat{B}\times[\vec{k}(t)-\vec{k}(0)]$$



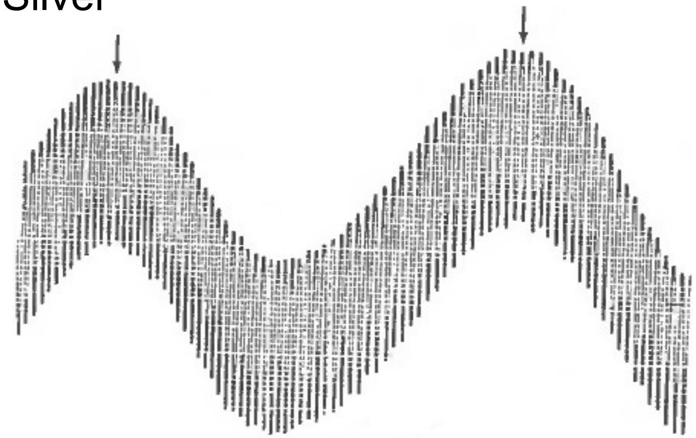
- *r*-orbit rotates by 90 degrees w.r.t the *k*-orbit and is scaled by λ_B^2

magnetic length: $\lambda_B \equiv (\hbar c/eB)^{1/2}$ (~ 256 A at B = 1 T).

- Higher BZ, Fermi surface
- Semiclassical electron dynamics
- de Haas-van Alphen effect

De Haas-van Alphen effect (1930)

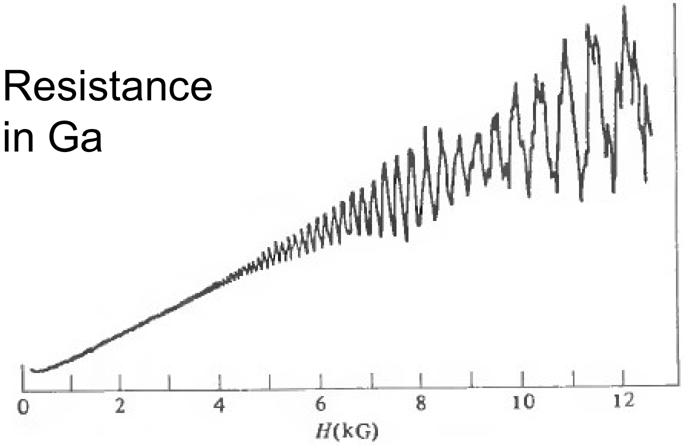
Silver



In a strong magnetic field, the magnetization of a crystal oscillates as the magnetic field increases.

Similar oscillations are observed in other physical quantities, such as

Resistance in Ga



- magnetoresistivity
(Shubnikov-de Haas effect, 1930)
- specific heat
- sound attenuation

… etc

These are all due to the quantization of electron energy levels in a magnetic field (Landau levels, 1930)

Quantization of cyclotron orbits

In the discussion earlier, the radius of a cyclotron orbit can be varied continuously, but the orbit should be quantized due to quantum effect.

- Bohr-Sommerfeld quantization rule (Onsager, 1952)

for a *closed* cyclotron orbit,

$$\oint d\vec{r} \cdot \vec{p} = \left(n + \frac{1}{2}\right) h$$

Why $(q/c)A$ is momentum of field? See Kittel App. G.

$$\text{where } \vec{p} = \vec{p}_{kin} + \vec{p}_{field} = \hbar\vec{k} + \frac{q}{c}\vec{A}, q = -e$$

$$\oint d\vec{r} \cdot \hbar\vec{k} = -\frac{e}{c}\oint d\vec{r} \cdot \vec{r} \times \vec{B} = 2\frac{e}{c}\Phi$$

also
$$\frac{e}{c}\oint d\vec{r} \cdot \vec{A} = \frac{e}{c}\Phi$$

$$\Rightarrow \Phi_n = \left(n + \frac{1}{2}\right)\frac{hc}{e}, \qquad A_n = \frac{\Phi_n}{B} = \left(n + \frac{1}{2}\right)2\pi\lambda_B^2$$

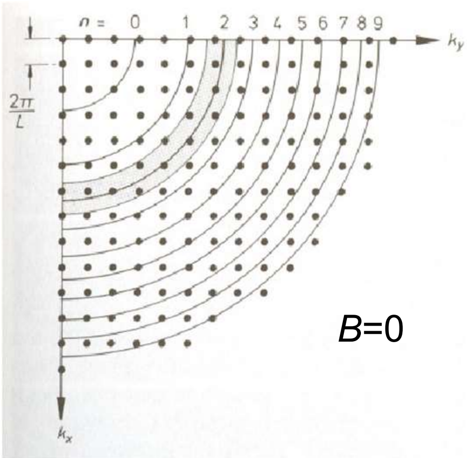
- The flux through an *r*-orbit is quantized in units of Φ_0.

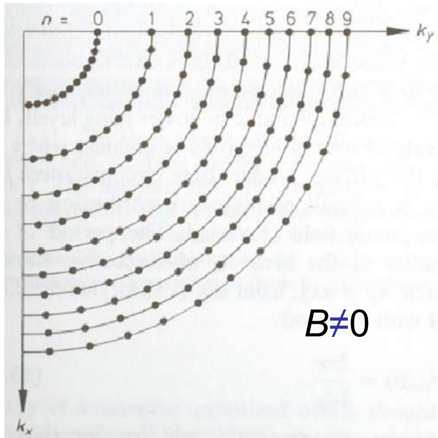
$\boxed{\text{flux quantum } \Phi_0 \equiv hc/e}$ (~ $4.14 \cdot 10^{-7}$ gauss · cm^2)

important

- Since a *k*-orbit (circling an area *S*) is closely related to a *r*-orbit (circling an area *A*), the orbits in *k*-space are also quantized (Onsager, 1952)

$$S_n = \frac{A_n}{\lambda_B^4} = \left(n+\frac{1}{2}\right)\frac{2\pi e}{\hbar c}B = \left(n+\frac{1}{2}\right)\frac{2\pi}{\lambda_B^2}$$





- Energy of orbits in 2D (for spherical FS)

$$\varepsilon_n = \frac{(\hbar k_n)^2}{2m} = \left(n+\frac{1}{2}\right)\hbar\omega_c$$

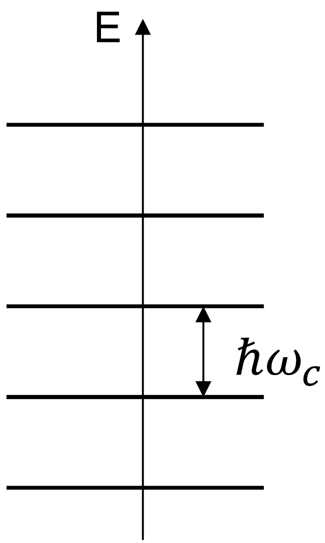
Cyclotron frequency

$$\boxed{\hbar\omega_c = \frac{eB}{mc}} \cong 1.16\cdot 10^{-4}\,[B/T]\ \mathrm{eV}$$

Landau levels (due to cyclotron orbits)

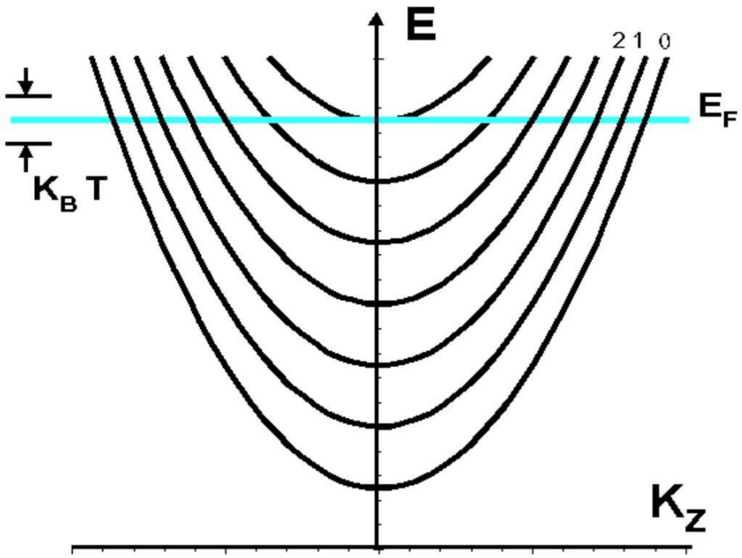
In 2D

$$\varepsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega_c$$

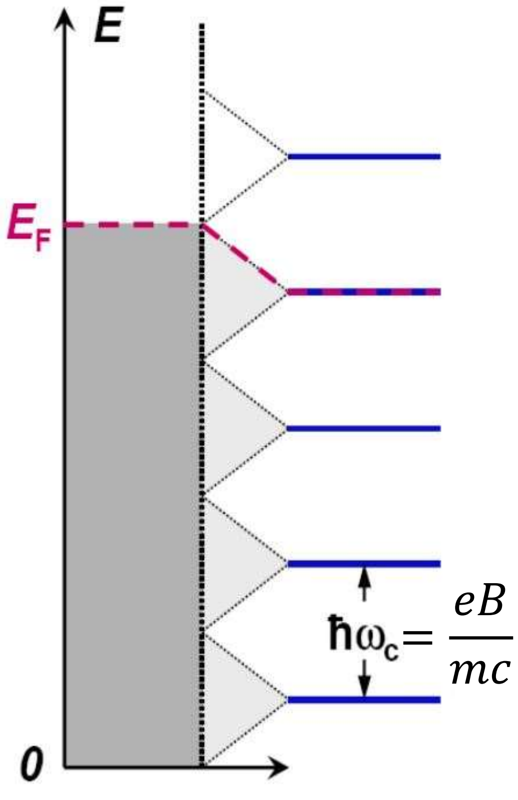


In 3D, the k_z direction is not quantized

$$\therefore \quad \varepsilon_{n,k_z} = \left(n + \frac{1}{2}\right)\hbar\omega_c + \frac{\hbar^2 k_z^2}{2m}$$



Degeneracy of Landau level

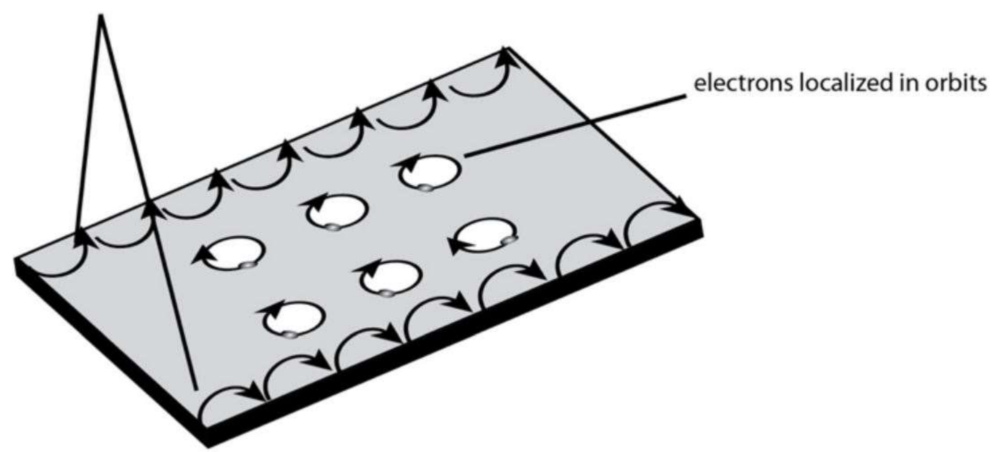


$$D = 2\frac{2\pi eB/\hbar c}{(2\pi/L)^2}$$

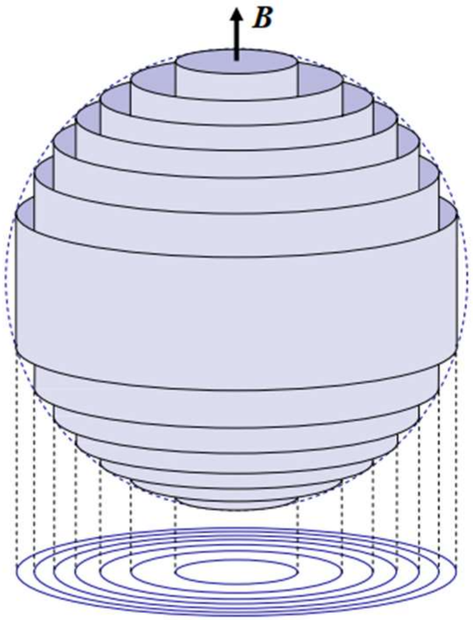
spin

$$= \frac{2BL^2}{hc/e} = 2\frac{\Phi_{\text{sample}}}{\Phi_0}$$

Highly degenerate



In the presence of B, the Fermi sphere becomes a stack of cylinders.



- Fermi energy $\sim$ 1 eV

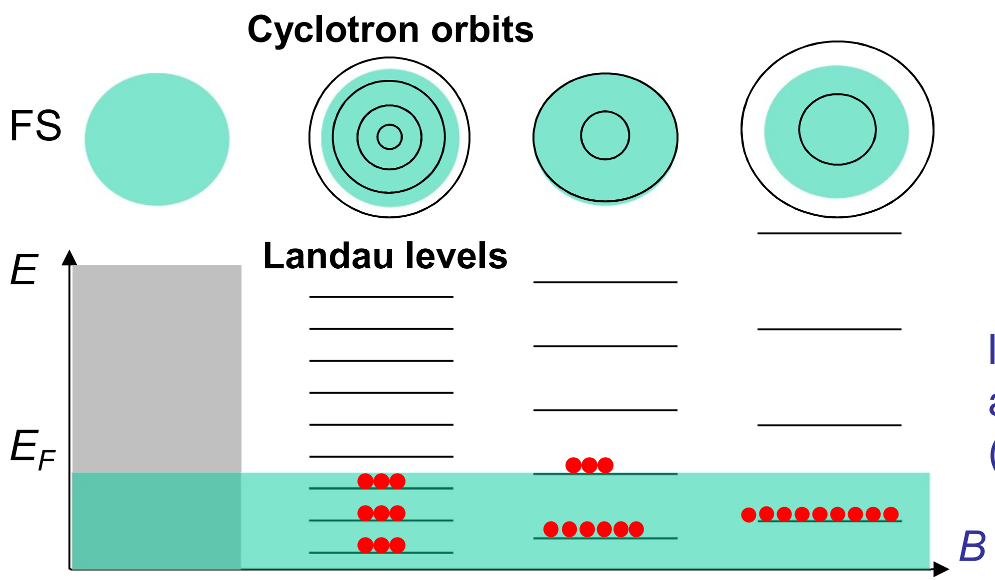
  cyclotron energy $\sim$ 0.1 meV (for B = 1 T)

  $\therefore$ the number of cylinders $\sim$ 10000
- need low T and high B to observe the quantization.

Hunklinger, Festkörperphysik

Radius of cylinders $\propto \sqrt{B}$, so they expand as we increase *B*.

The orbits are pushed out of the FS one by one.



larger level separation, and larger degeneracy (both $\propto$ *B*)

- Successive *B*'s that produce orbits with the same area:

equal increment of 1/*B* reproduces similar orbits

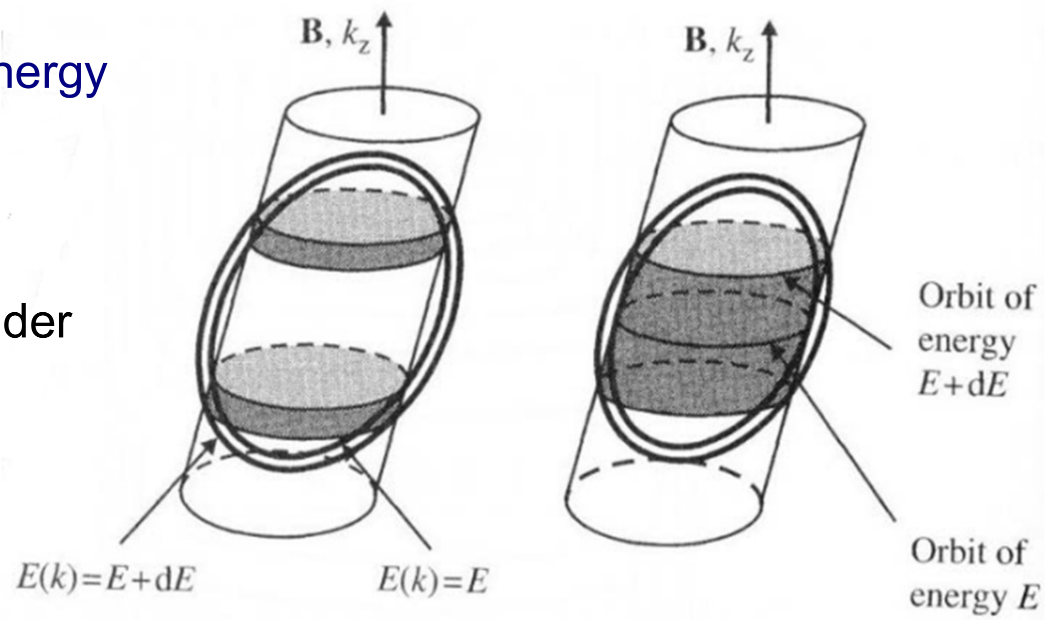
$S_n = (n+1/2)\, 2\pi e/\hbar c\, B$

$S_{n-1}' = (n-1/2)\, 2\pi e/\hbar c\, B'$ ($B' > B$)

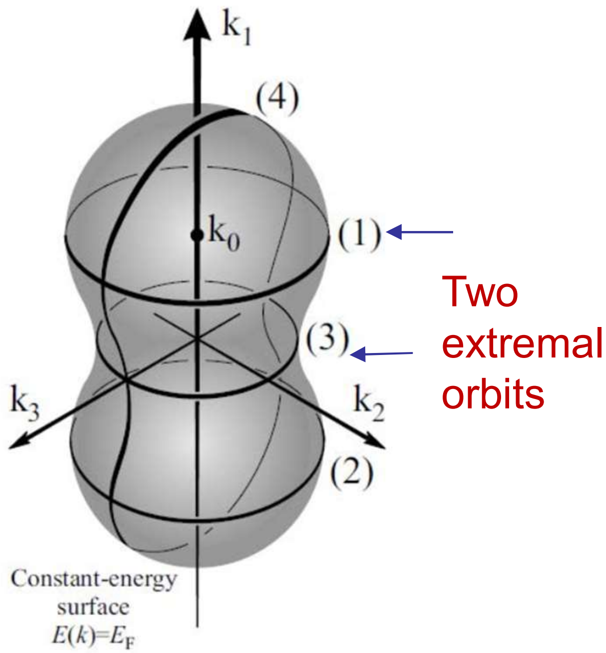
$$\rightarrow \boxed{S\left(\frac{1}{B}-\frac{1}{B'}\right)=\frac{2\pi e}{\hbar c}}$$

Oscillation of DOS at Fermi energy

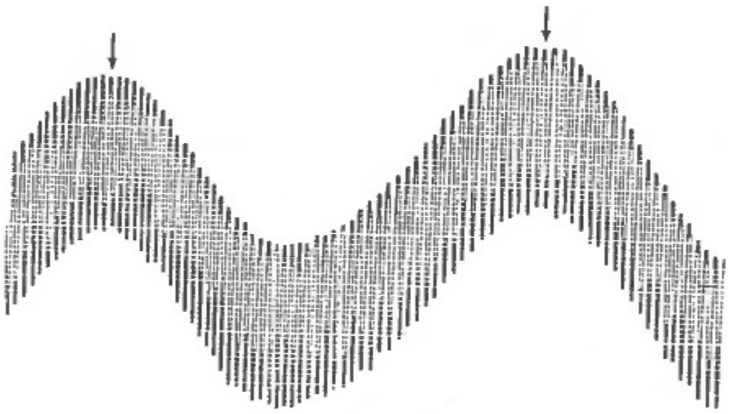
- Number of states in $d\varepsilon$ are proportional to area of cylinder in an energy shell.



- Number of states at E_F is highly enhanced when there is extremal orbit on FS.
- There are extremal orbits (and enhanced DOS) at regular interval of $1/B$.
- This oscillation of DOS (in $1/B$) can be detected in any physical quantity that depends on DOS .



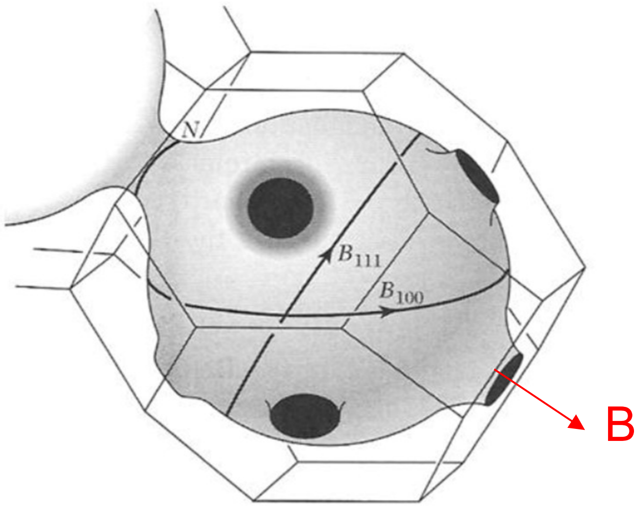
Determination of FS

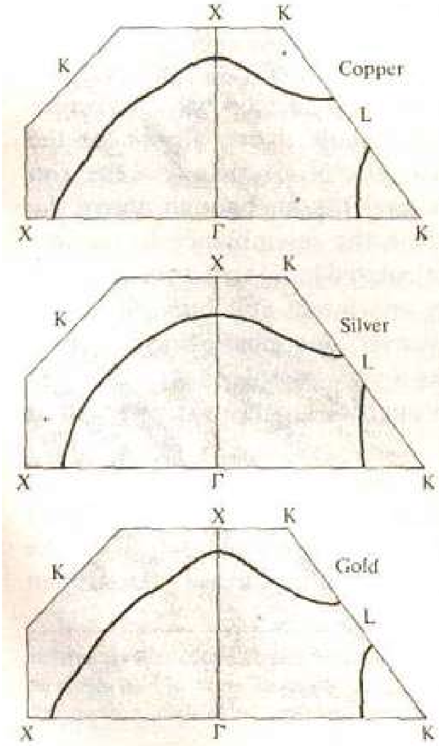


In the dHvA experiment of silver, the two different periods of oscillation are due to two different extremal orbits.

Recall that $S_e\left(\frac{1}{B}-\frac{1}{B'}\right)=\frac{2\pi e}{\hbar c}$

Therefore, from the two periods we can determine the ratio between the sizes of "neck" and "belly“.





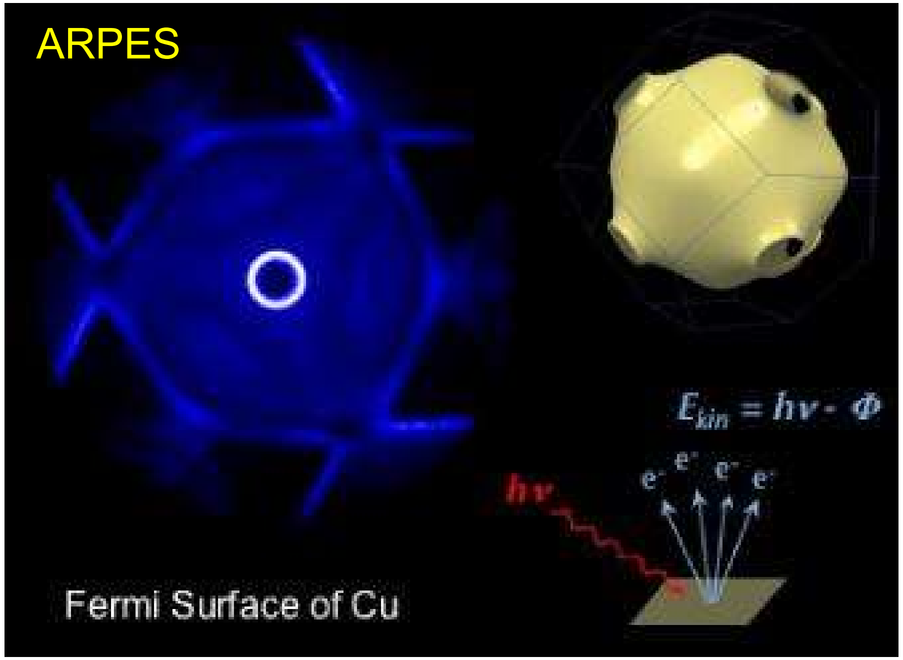
A_{111}(belly)/A_{111}(neck)=27

A_{111}(belly)/A_{111}(neck)=51

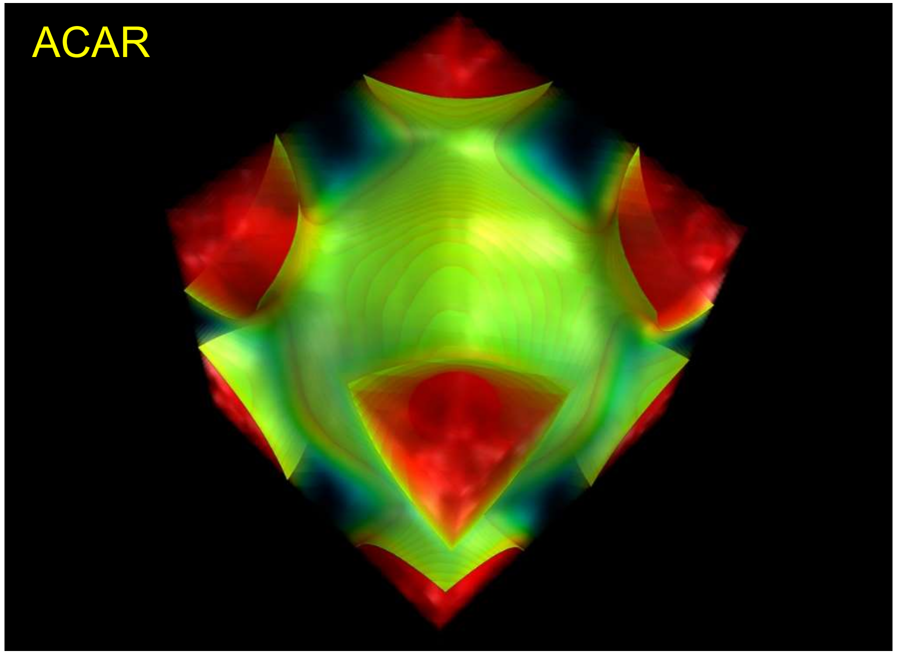
A_{111}(belly)/A_{111}(neck)=29

Determination of FS

- dHvA
- ARPES (Angle-resolved photoemission spectroscopy)
- ACAR (Angular Correlation of Electron-Positron Annihilation Radiation)
- …



F.Baumberger's webpage



Fermi surface and electron momentum density of Copper (wiki)