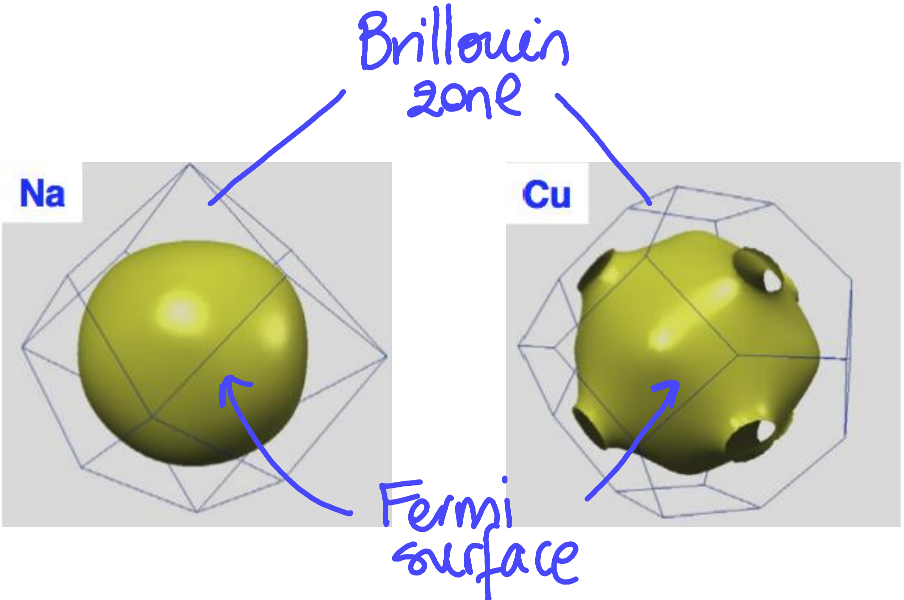
A bit more about Fermi surfaces

Recap

<u>Fermi surface</u> is the surface of constant energy E_F in $\vec{k}$-space.

at $T = 0K$, Fermi surface separates the unfilled orbitals from filled ones.

! electrical properties of metals are determined by the volume and shape of Fermi surfaces.



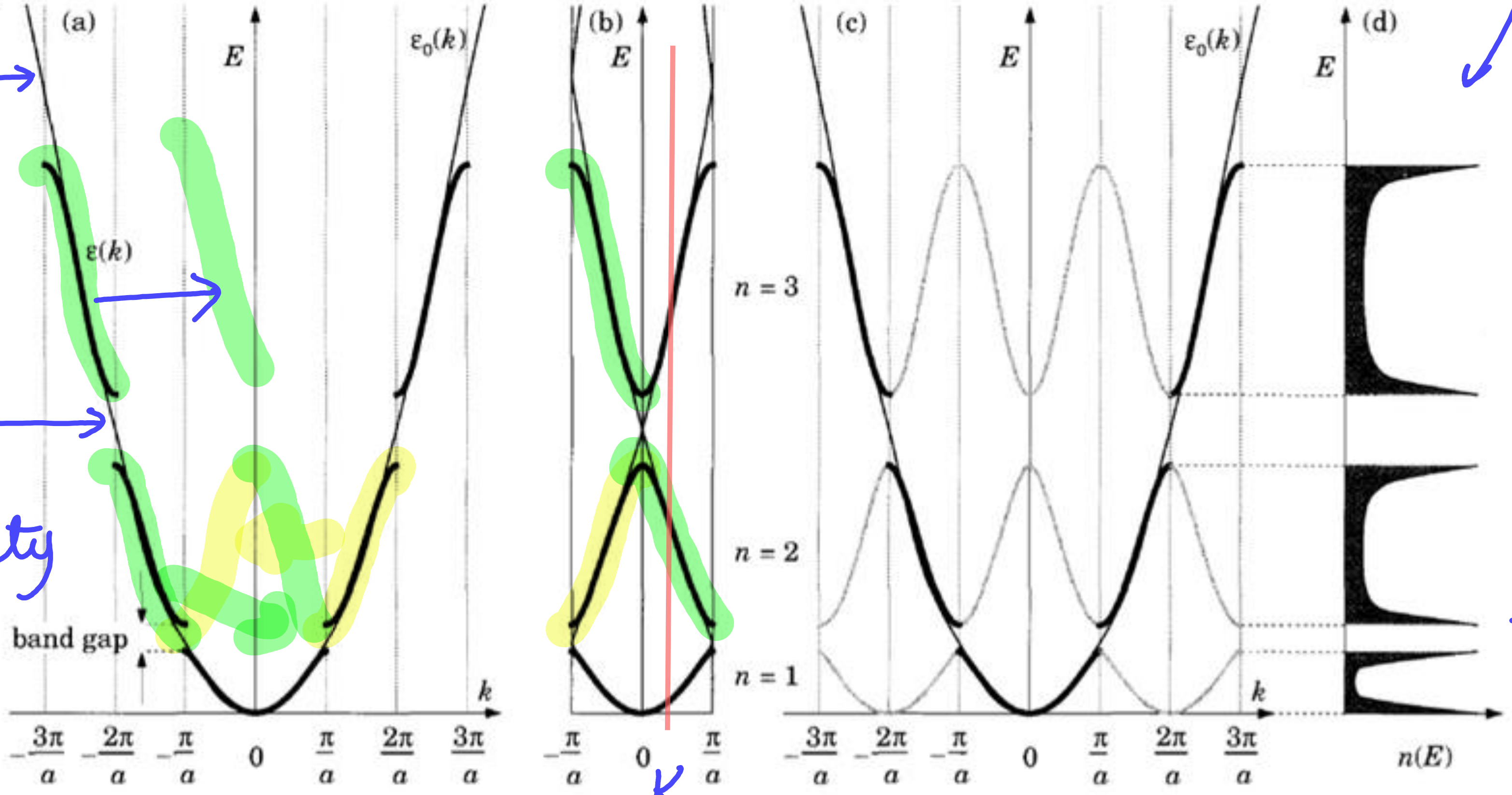
Recap

Extended - Reduced - Periodic zone scheme

Density of states

Free e⁻

open of a gap due to lattice periodicity



2 wavefunctions at same K but ≠ E are independent

⇓

the wavefunctions will be made of ≠ plane wave components c_n

1st B.Z

K

In reduced scheme, we may have ≠ energies at same K-value

→ each ≠ energy characterize a band $\underline{n}$

Bloch theorem

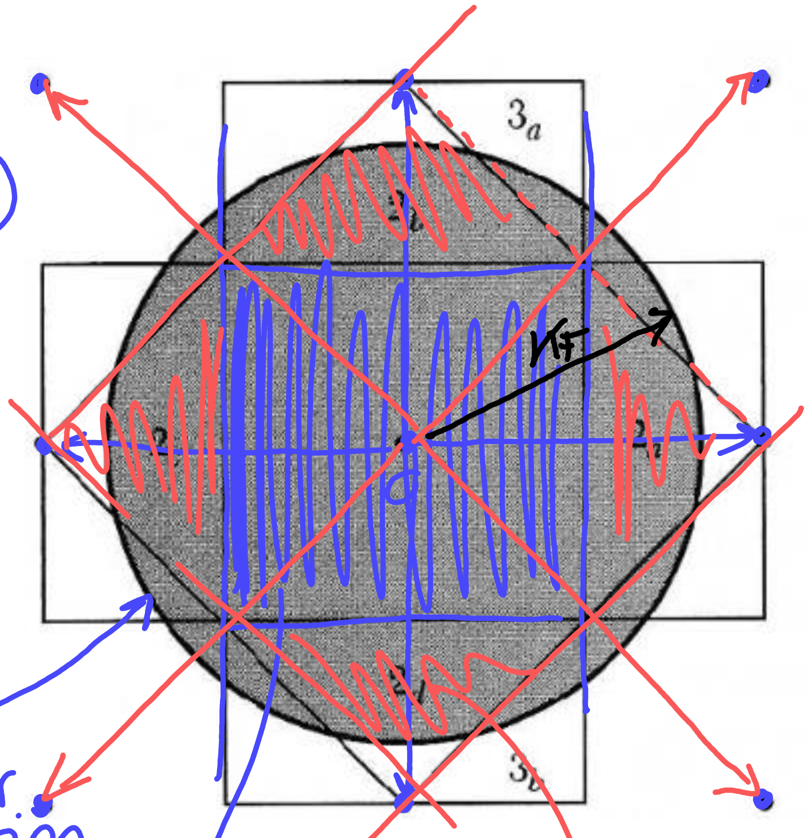
$$\psi_{n,K} = \exp(i\bar{K}\bar{r})\, u_{nK}(\bar{r}) = \sum_G c_{\underline{n}}(K+G)\exp\left(i(\bar{K}+\bar{G})\cdot\bar{r}\right)$$

band index n

Recap

Brillouin zones of a square lattice

(reciprocal lattice)



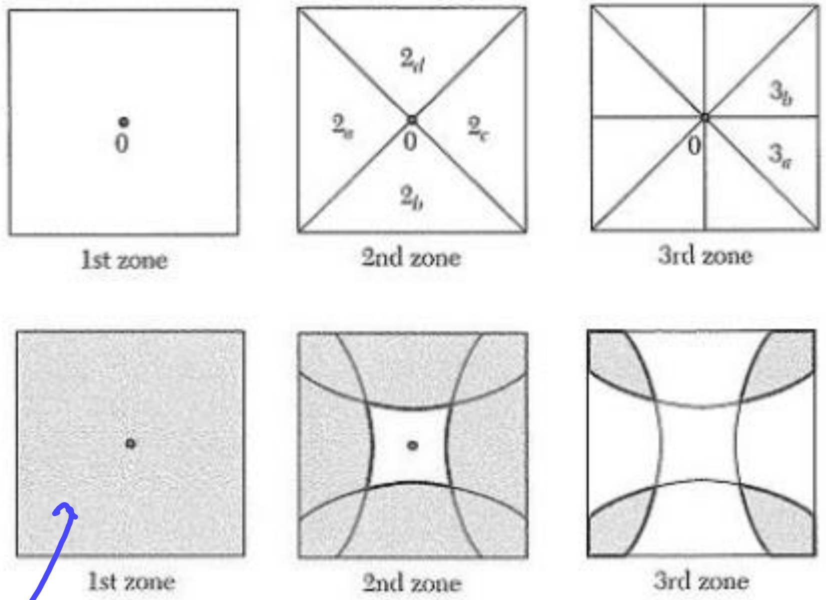
Fermi surface for some particular concentration of electrons

(Remember that previously we studied in detail the cases of N & 2N e^-)

1rst B.Z

2nd B.Z

Mapping of 1,2,3 B.Z. in the reduced zone scheme

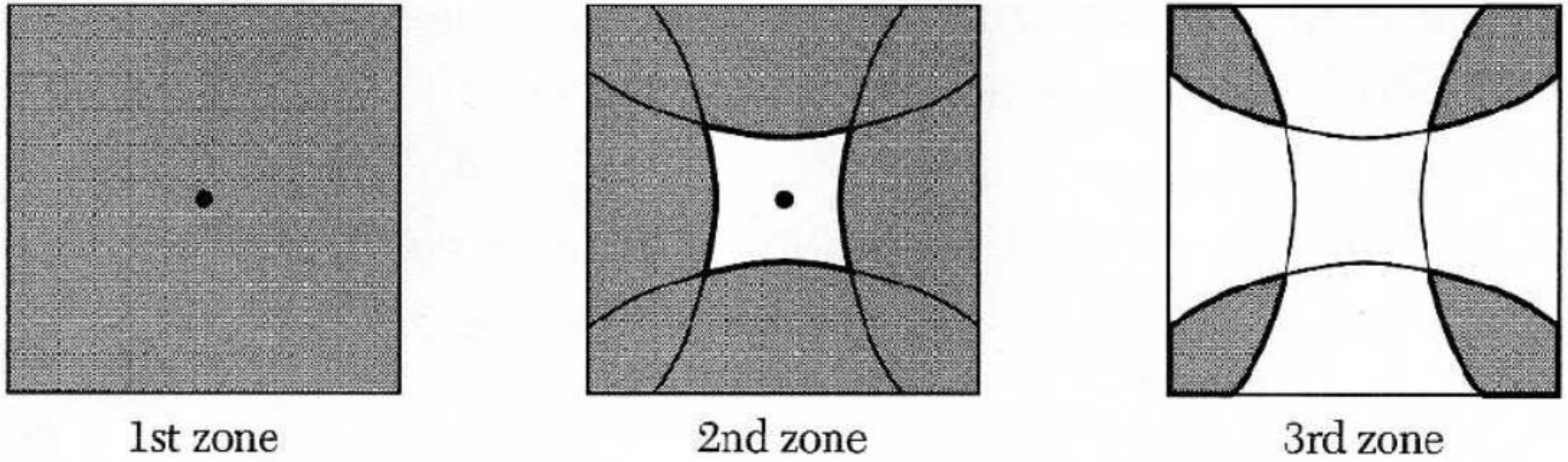


filled

Free e- Fermi surface viewed in reduced zone scheme.

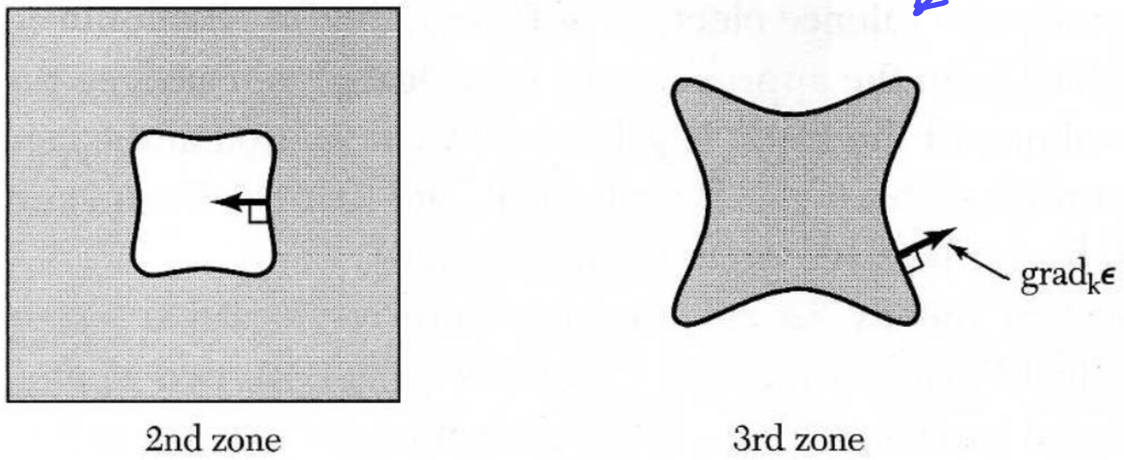
Recap

Free e- model



Effect of nearly free e- model

(the crystal potential tends to round the corners in the Fermi surfaces)

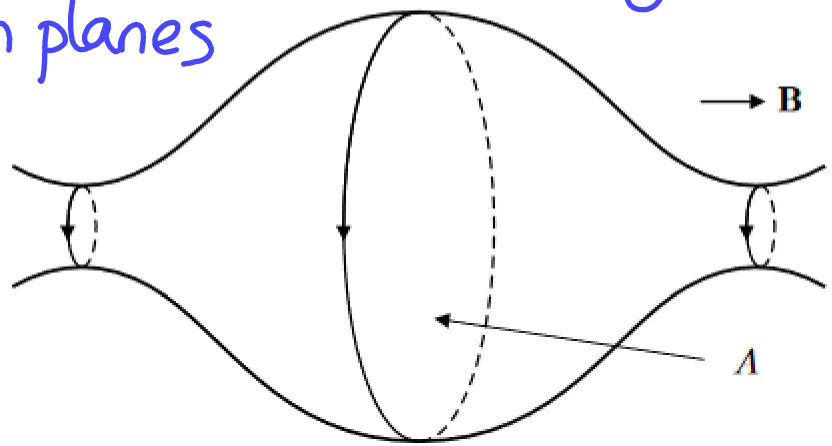


Recap Back to magnetic field experiments :

Effect of external B on a band e- : $\hbar \frac{d\bar{k}}{dt} = -e\bar{v} \times B$

- $v = \frac{1}{\hbar} \nabla_k E(k) \longrightarrow \frac{dk}{dt} \perp \nabla_k E(k)$: e- path (orbit) is one of constant energy

- in k-space, the possible e- orbits are thus described by intersections of surfaces of constant energy with planes $\perp$ to B.



→ an e- on a Fermi surface will move on a curve on the Fermi surface

Figure 9.2: Orbits on a Fermi surface section are in planes perpendicular to **B**. Here, A represents the k-space cross-sectional area of the orbit.

Electron orbits, hole orbits and open orbits

Guess each one!

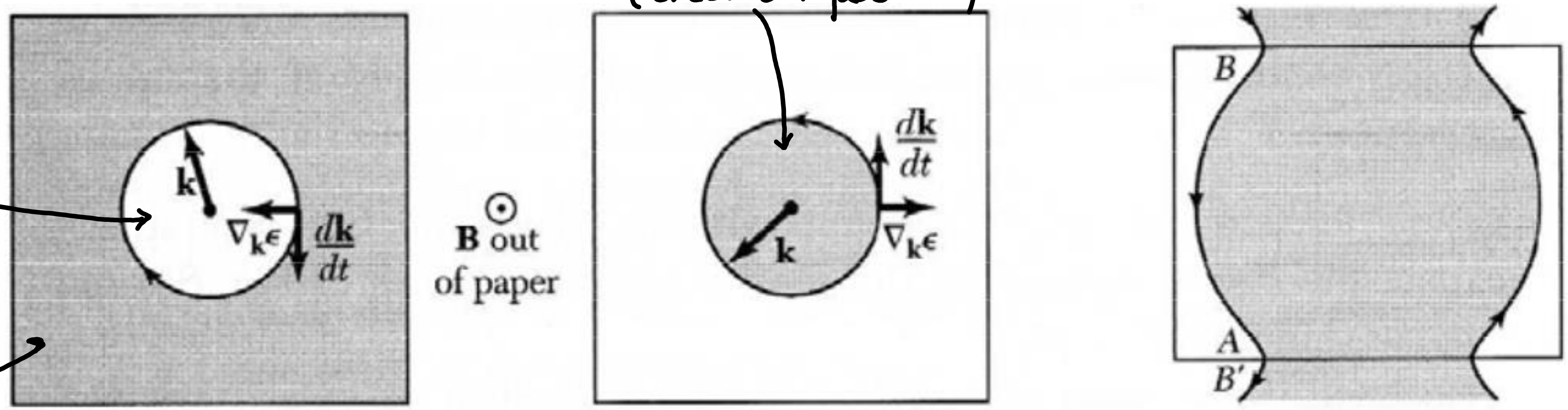
3 types of orbits in a magnetic field:

hole-like orbit

electron-like orbit (electron pocket)

open-orbit

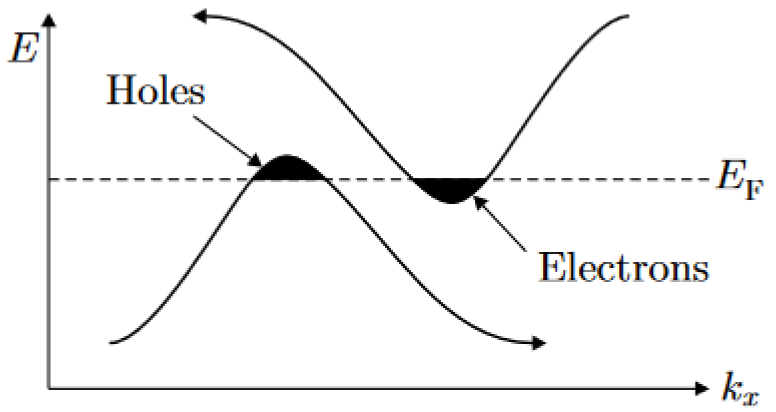
hole pocket



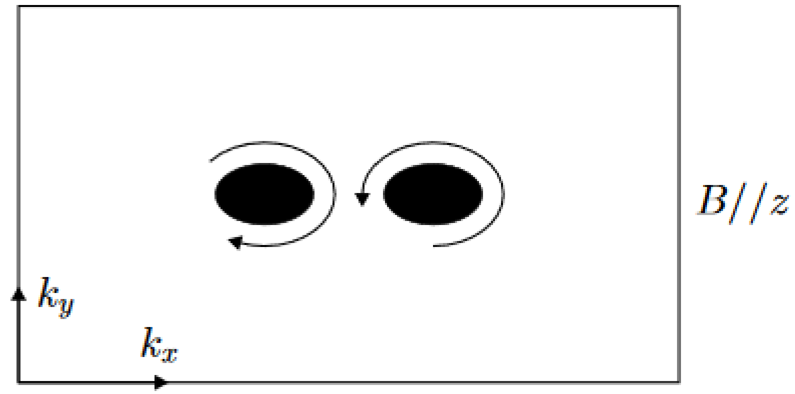
filled states

When particle reaches boundary at A, it goes back to B

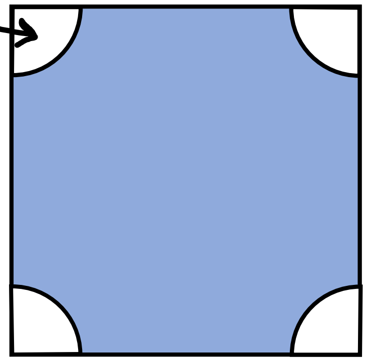
2 bands crossing Fermi surface



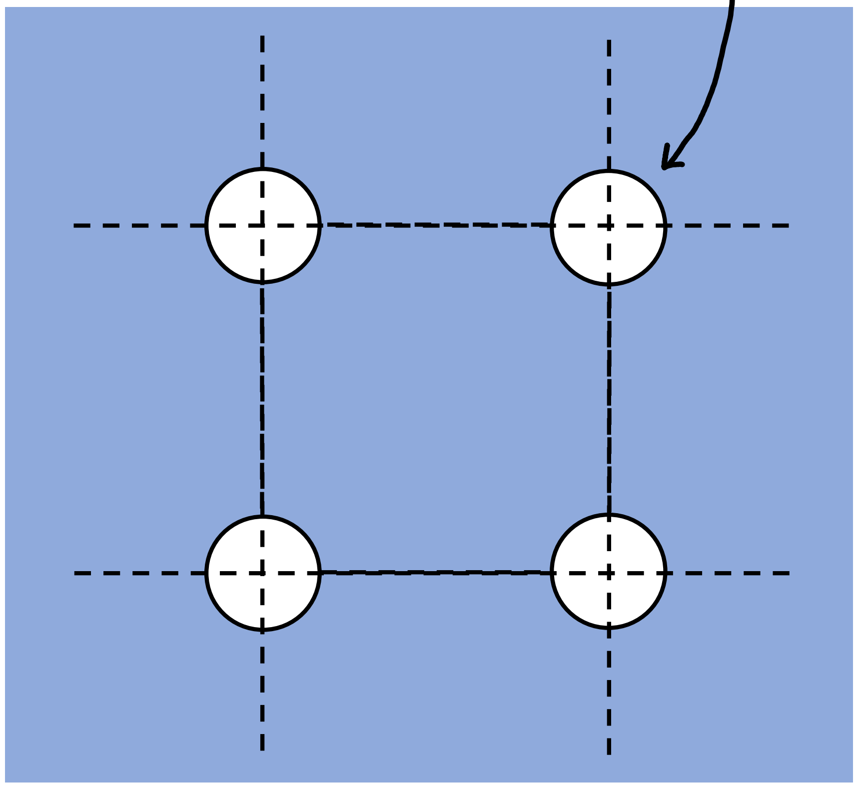
Fermi surface cross-section

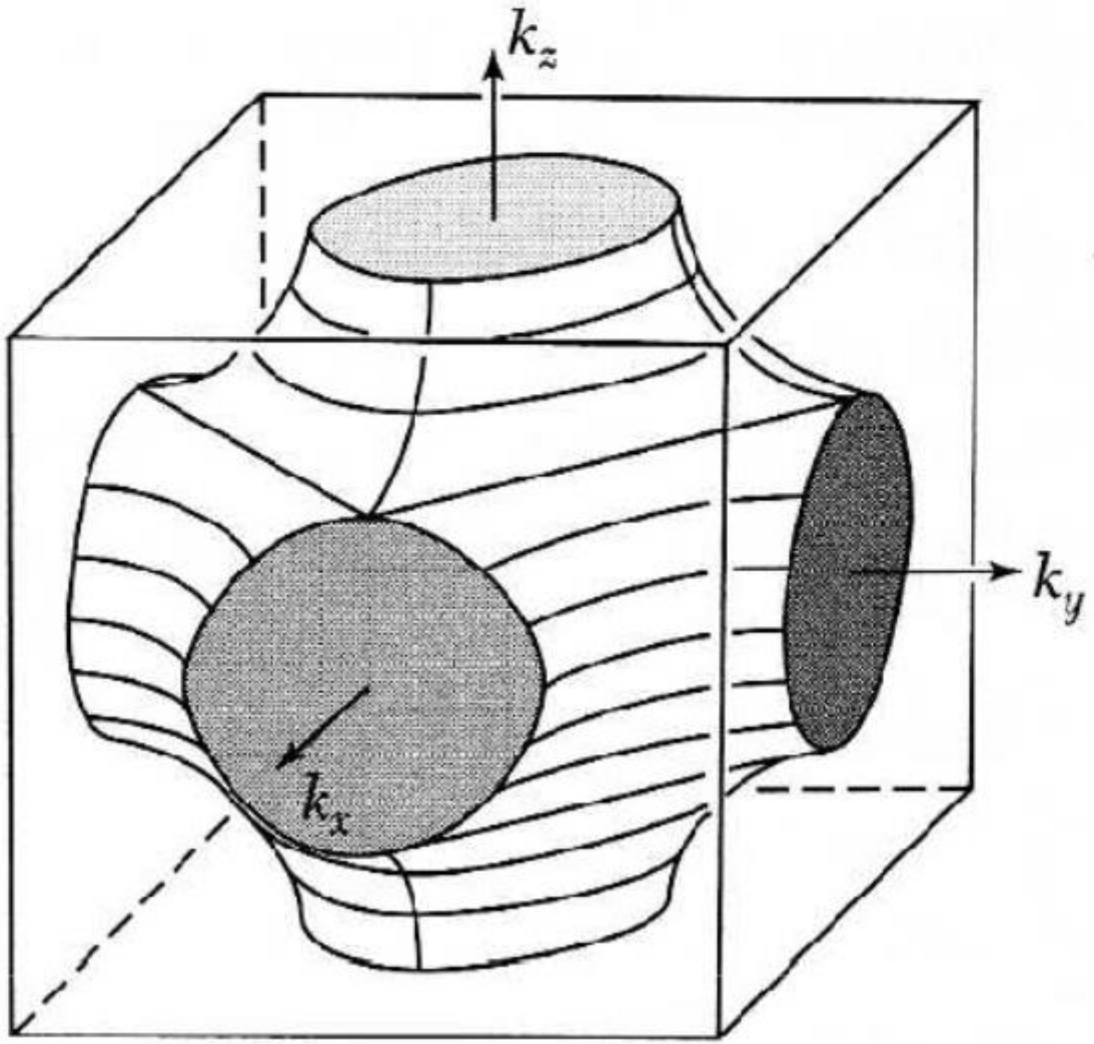


vacant states at the corners



in periodic zone scheme it is easy to see that each circle forms a hole-like orbit





We can cut a plane in the 3D reduced zone. Depending on which plane we cut, we may find an electron orbital, a hole orbital or an open orbital in the figure above.

Experimental methods to determine Fermi surfaces

- Magnetoresistance
- Anomalous skin effect
- Cyclotron resonance
- Magneto-acoustic geometric effects
- Shubnikov-de Haas effect
- de Haas-van Alphen effect

⋮

etc.

Quantization of orbits in a magnetic field

Bohr - Sommerfeld relation : orbits in a magnetic field are quantized.

$$\oint \bar{p} \cdot d\bar{r} = (n+\gamma)\, 2\pi\hbar$$

integer

phase correction (i.e. $\gamma = \frac{1}{2}$ for e-)

$$\vec{p} = \bar{p}_{kin} + \bar{p}_{field} = \hbar\bar{k} + q\bar{A}$$

charge

$\bar{B} = \nabla \times A$

[... Kittel Ch. 9 ...]

$$\oint \bar{p} \cdot d\bar{r} = -e\underbrace{\Phi}_{\text{Flux contained within orbit in real space}} = (n+\gamma)\, 2\pi\hbar$$

$$\Rightarrow \boxed{\Phi_n = (n+\gamma)\, \frac{2\pi\hbar}{e}}$$

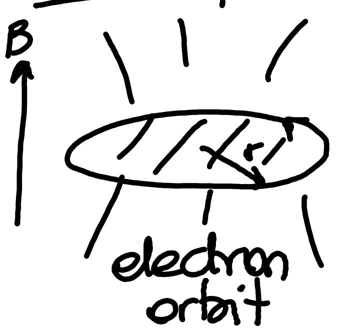
We are interested in orbits in K-space.

$$\hbar \frac{dK}{dt} = e \frac{dr}{dt} \times B$$

$$\Delta r = \frac{\hbar}{eB} \Delta K$$

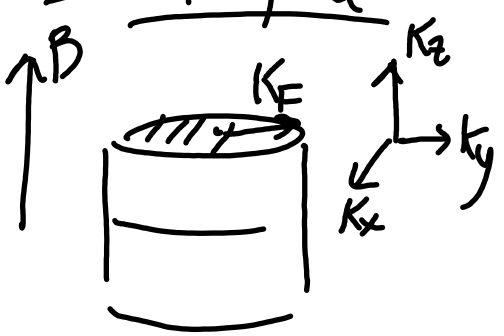
$$A_n = \left(\frac{\hbar}{eB}\right)^2 S_n$$

Real space



Area enclosed
$A = \pi r^2$

Reciprocal space



Fermi surface area
$S = \pi K_F^2$

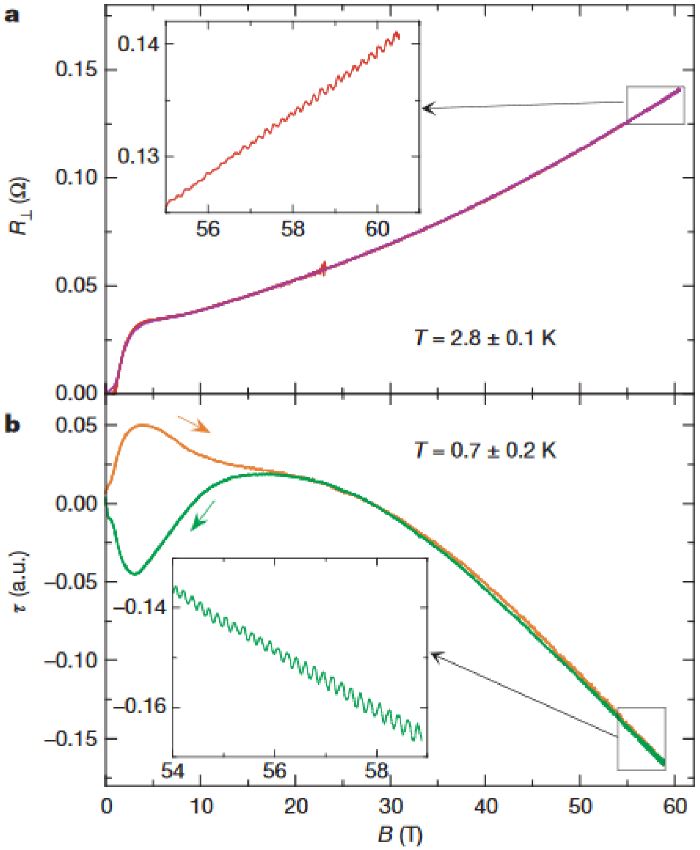
$$\Rightarrow \quad \Phi_n = \left(\frac{\hbar}{e}\right)^2 \frac{1}{B} S_n = (n+\gamma)\left(\frac{2\pi\hbar}{e}\right)$$

$$\Rightarrow \quad S_n = (n+\gamma)\left(\frac{2\pi\hbar}{e}\right)$$ $\leftarrow$ Area of an orbit in K-space

$$S\left(\frac{1}{B_{n+1}} - \frac{1}{B_n}\right) = \frac{2\pi e}{\hbar}$$ $\Rightarrow$ equal increments of $1/B$ lead to similar orbits

- Population of orbits at E_F oscillates with B
- Oscillatory effects on $1/B$ often observed: ρ, χ, C...

Quantum oscillations



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$Tl_2Ba_2CuO_{6+x}$

Shubnikov-de Haas effect =
Quantum oscillations with resistivity

De Haas–van Alphen effect =
Quantum oscillations with magnetic susceptibility

De Haas – van Alphen Effect

- = oscillation of the mag. moment of a metal as function of applied B.
- Effect observed at low T and strong B

2D) we know : - area of an orbit in K_x, K_y space is quantized
- area between to successive orbits $\Delta S = S_n - S_{n-1} = \frac{2\pi e B}{\hbar}$

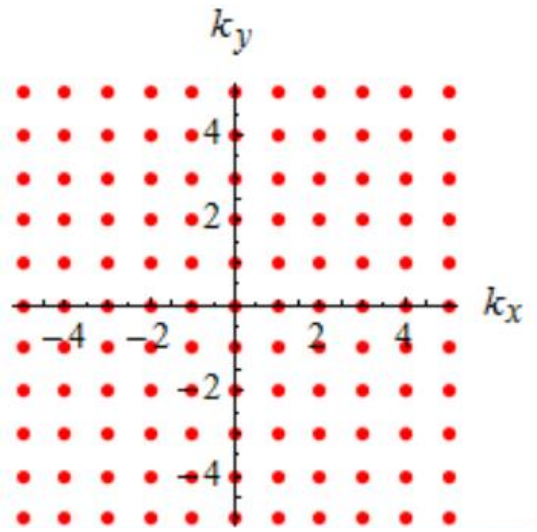
Reminder: area in K-space occupied by 1 orbital $= \left(2\pi/L\right)^2$
(not considering spin)

The number of free e orbitals that now will merge in a single mag. level:

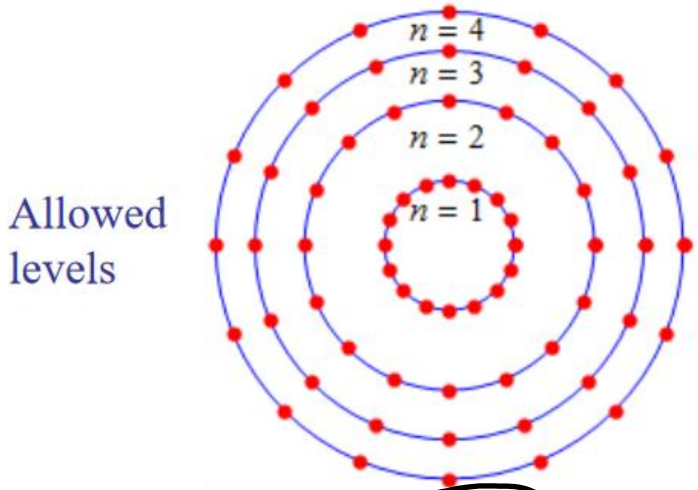
$$D = \frac{\frac{2\pi e B}{\hbar}}{\left(\frac{2\pi}{L}\right)^2} = \underbrace{\frac{e L^2}{2\pi \hbar}}_{\rho} B$$

LANDAU LEVELS
(quantization of cyclotron orbits of charged particles in a magnetic field)

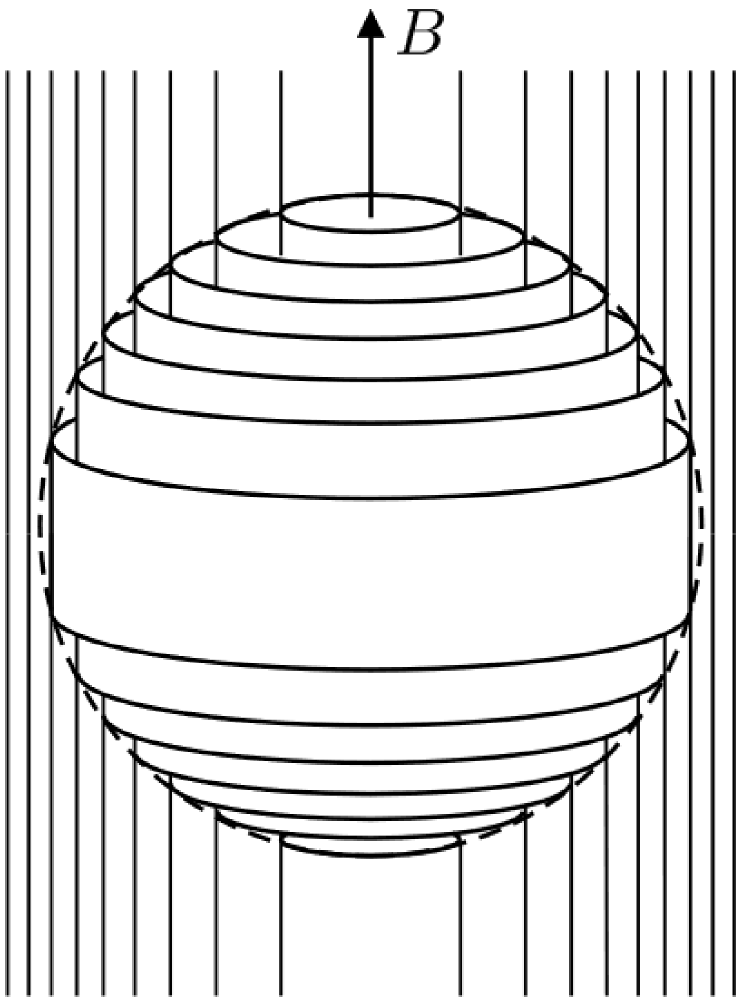
(notice that degeneracy D changes with B)



$B = 0$



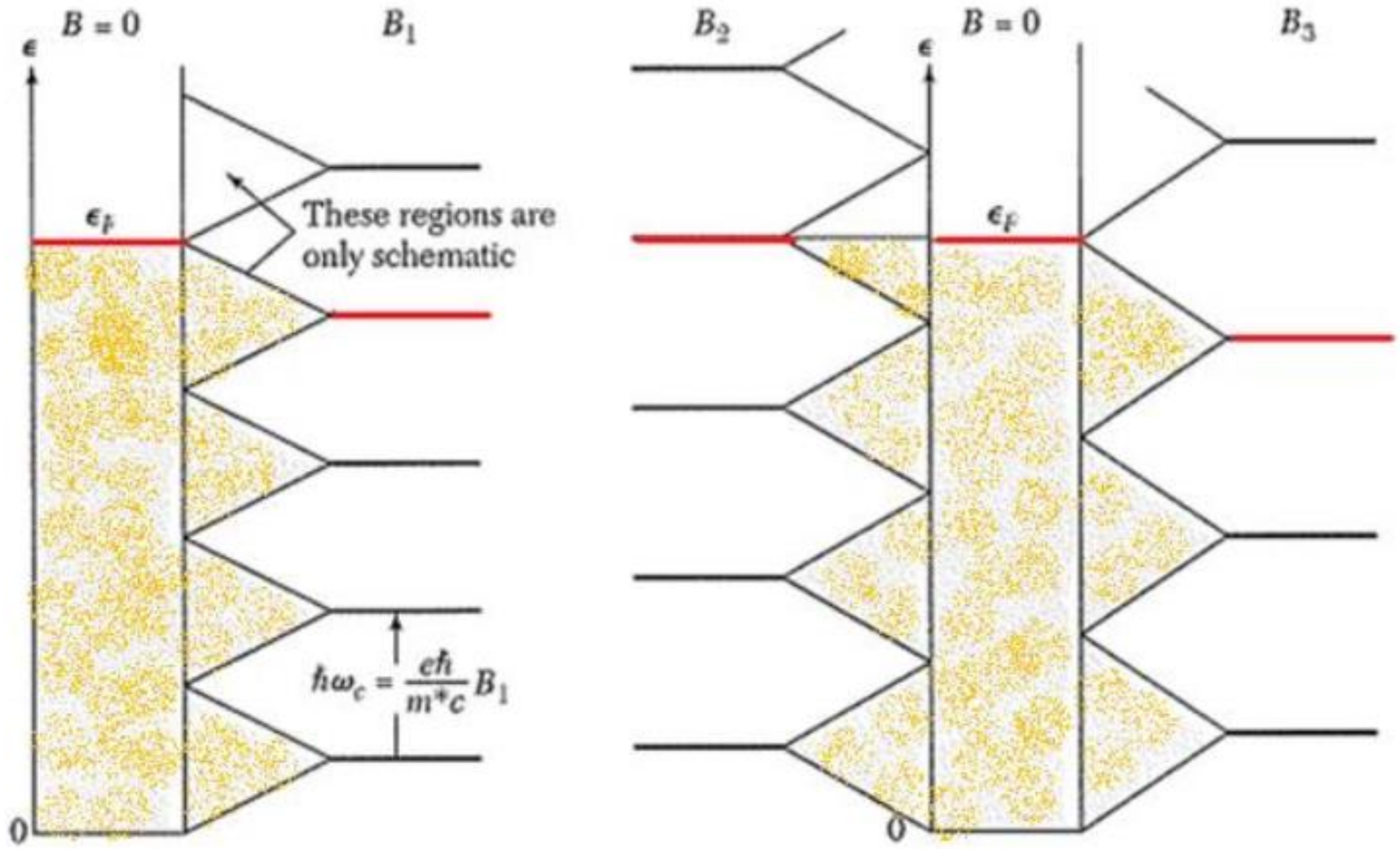
$B \neq 0$



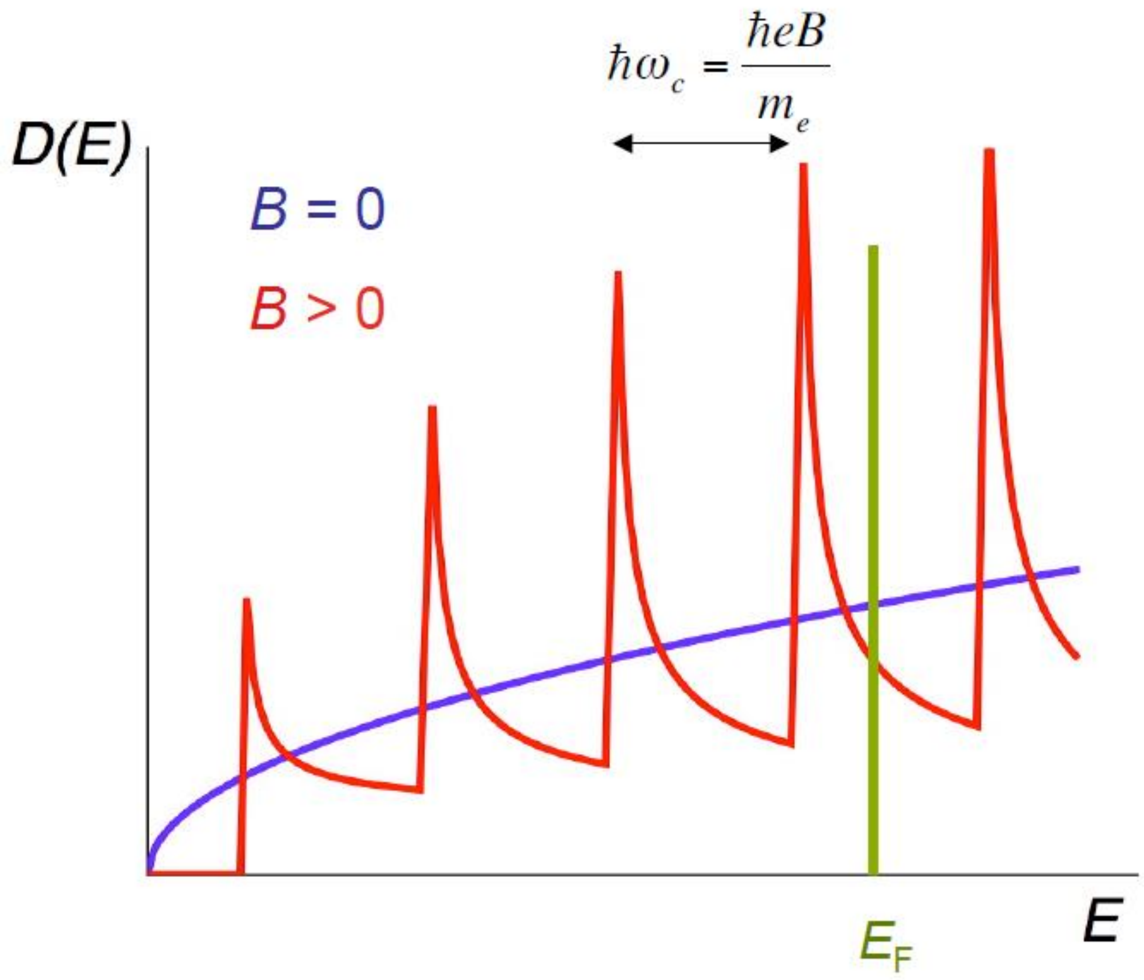
Schematic of a Fermi sphere rearranged into Landau tubes.

dHvA effect
for a free e- gas
in 2D in B

The total energy
is min at $B_1, B_3 \ldots$
and max at $B_2 \ldots$



Density of states is an "∞-ladder" of Landau levels



Oscillations occur at equal intervals $1/B$:

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar S}$$

Extremal area of Fermi surface $\perp B$

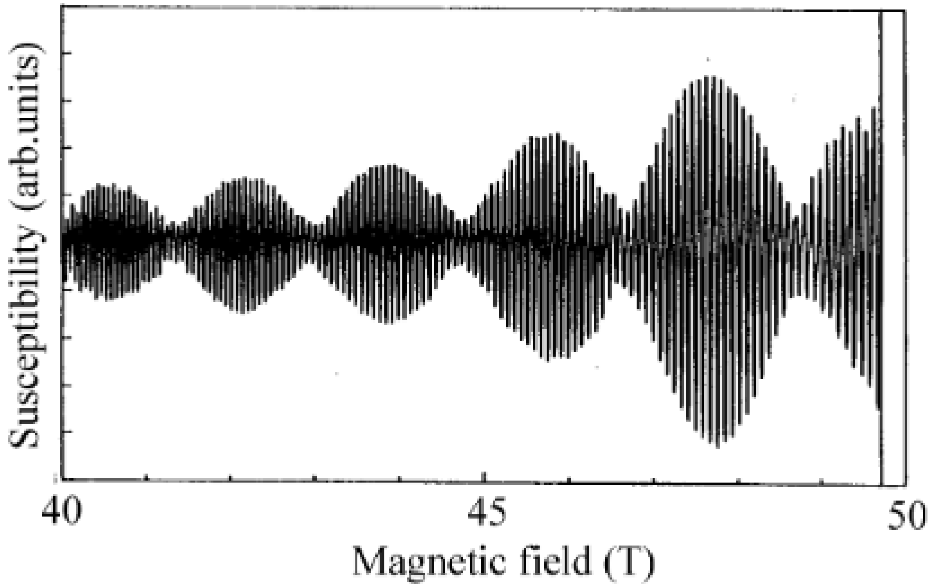


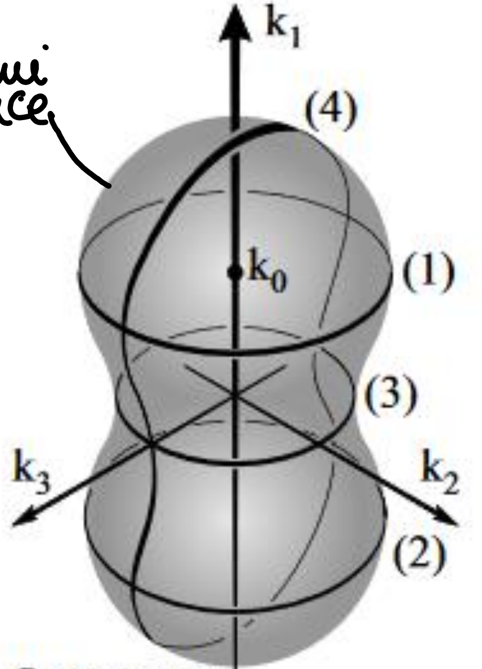
Figure 9.9: de Haas-van Alphen oscillations in Pt at 4.2 K with **B** parallel to [111]. The data have been recorded using a pulsed magnetic field. Note the presence of two frequencies of oscillations due to two extremal orbits about the Fermi surface. The y axis, labelled "susceptibility", represents the voltage V induced in the coil divided by $(\mathrm{d}B/\mathrm{d}t)$, leaving a quantity proportional to the differential susceptibility $(\mathrm{d}M/\mathrm{d}B)$ (Data from S. Askenazy, Physica B **201**, 26 (1994).)

Extremal orbits

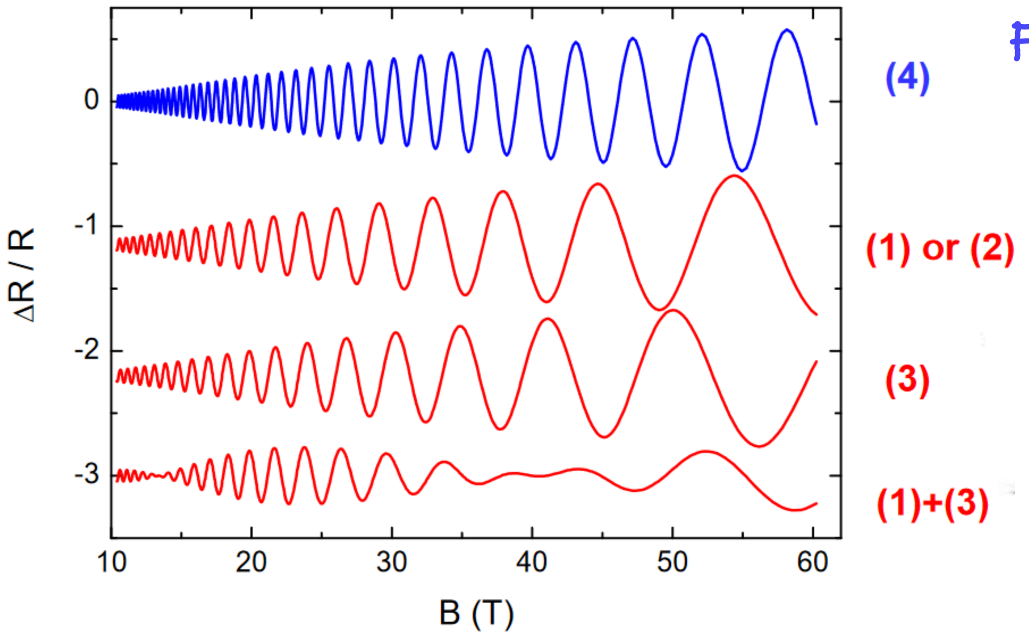
- they determine the periodicity of quantum oscillations
- their periods are stationary with respect small changes in k_B (k_B = component of k along mag. field)

For $\bar{B} \parallel k_1$, there will be 3 extremal orbits : (1), (2), (3)
since (1) & (2) have same area → 2 series of quantum oscillations (i.e. 2 frequencies)

Fermi surface

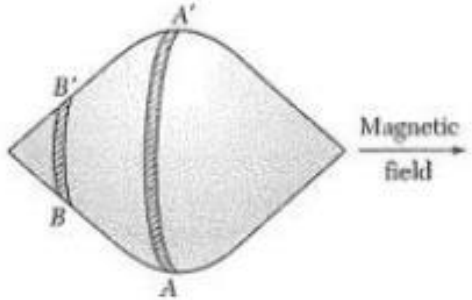


Constant-energy surface $E(k)=E_F$

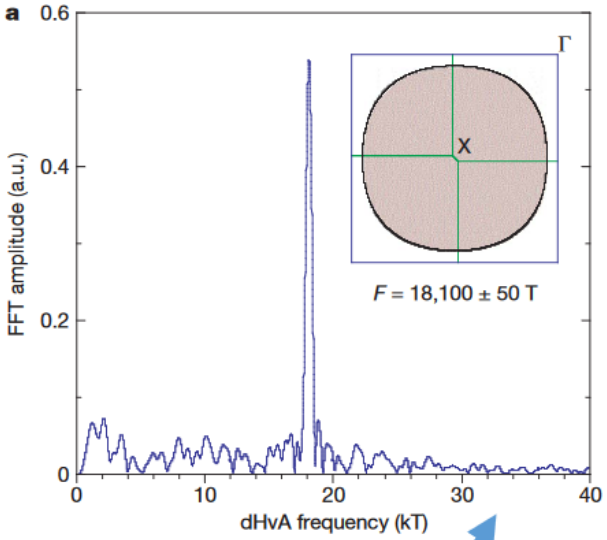


(4) F=500 T
(1) F=250 T
(3) F=230 T

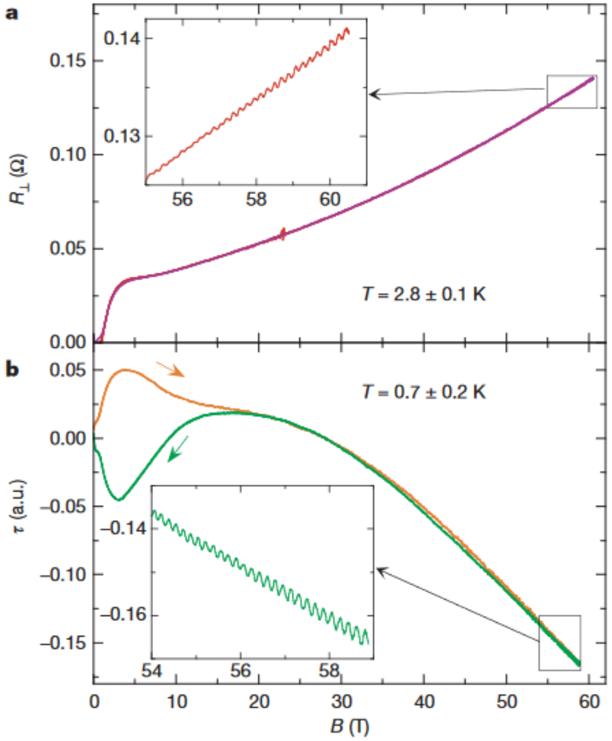
For $\bar{B} \parallel k_2$, only one extremal orbit : (4)



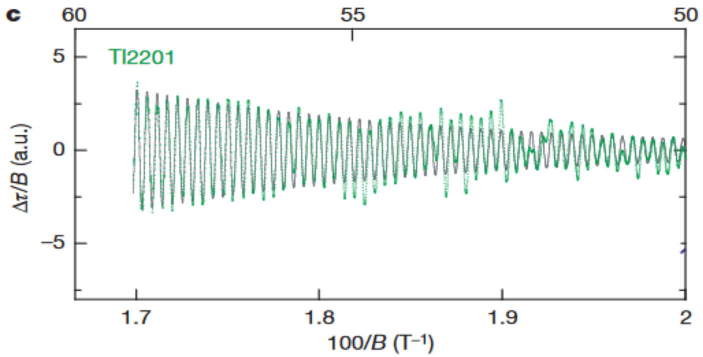
(c) Fourier Transform



(a) RAW DATA



(b) OSCILATIONS VERSUS 1/B



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