Dynamics of electrons in external field

- The motion of electrons is defined by the shape of it's Fermi surface.

- i.e. for each point on the $E_i(\bar{p}) = E_{i,Fermi}$ we need to know the dispersion curve for a given direction.

- Almost always we can consider the motion in a quasi classical limit b/c
  $$\lambda_B \sim 2\pi\hbar/p_F \quad \text{with} \quad p_F \sim \frac{2\pi}{a}\hbar \quad \text{we get}$$
  $$\lambda_B \sim a \quad , \text{while the mean free path}$$
  for e^- is $\gg a$.

- Group velocity of e^- is always $\perp$ to the $E_i(p)$: $\dfrac{\partial E}{\partial \bar{p}} = \bar{v} = \nabla_p E$
  and in general is non-collinear to its momentum.

  Lets study the case when we apply electric field $\bar{E}$ when $T=0K$ (no scattering off phonons). Lets assume the direction of $\bar{E} \parallel [001]$

  Lets assume we have only one e^- at the zone center: Γ point, where $p=0$ and $K=0$

  how I turn on the field $\bar{E}$
  and my e^- experiences $\bar{F} = -e\bar{E}$
  and $p = |e| |E| \cdot t$

if I have had a free electron then the momentum would keep growing.
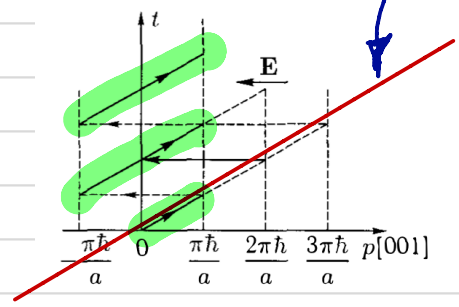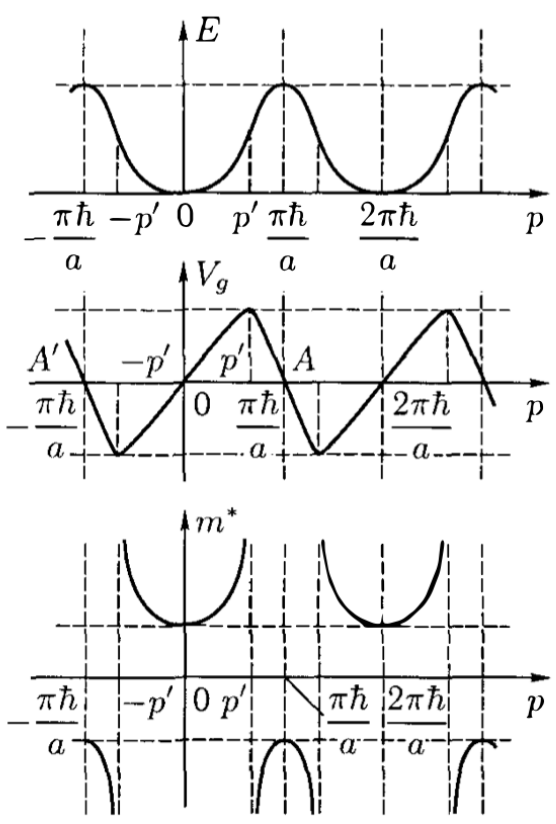
But in the crystal all is changed!
We have crystal field meaning that
$$\left(-\frac{\pi\hbar}{a}, 0\right) \text{ and } \left(\frac{\pi\hbar}{a}, \frac{2\pi\hbar}{a}\right)$$
are physically equal.

So we can translate the regions which are outside of $\left[-\frac{\pi}{a}\hbar \; ; \; \frac{\pi}{a}\hbar\right]$ by the crystal momentum we can get a set of curves all sitting in the 1st zone.

i.e. when electrons reach the boundary $p = \pm\frac{\pi\hbar}{a}$ its quasi momentum jumps into an opposite number, or

we could say the electron mirror refeects from the zone boundary.

what happens to the velocity is very strange.

$\upsilon = \dfrac{\partial E}{\partial p}$ and so is the kinetic energy of e^-

are periodic functions of $\bar{p}$ with the

period of $\dfrac{2\pi h}{a}$. So by taking derivative

$\dfrac{\partial E}{\partial p}$ we get υ_g (see figure on the previos page)

Now lets return to our problem of e^- in $\bar{E}$
Since $\bar{\upsilon}$ ‖ p $|\upsilon|$ is not proportional $|p|$
Since as $p \to \dfrac{\pi h}{a}$ $\upsilon \to 0$

- Note for positive p and positive υ
   we have motion to the right
      and for $-p$ $-\upsilon$ to the left.

   in other words the periodic motion in
   the p-space we can have a periodic
   motion in the real space.

-Physical meaning: while at I p is small
and the electron is free like

   when we apply E the momentum $\uparrow$
   and $l_B \downarrow$, and thus the electron
   is getting close to the zone boundary.

And at some $|p|$ it reaches the zone boundary where $v=0$

After that the reaction of lattice is stronger than $-e\bar{E}$ and at $p=\frac{\pi \hbar}{a}$ the momentum changes its sign and the electron jumps from $A \longrightarrow A'$ and

now the electron moves to the left against the external force and its $|p|$ gets reduced and as e^- moves away from the BZ it experience less crystal reaction and at some point p' it gets pushed to Γ point by $-e\bar{E}$

where the electron velocity changes its sign.

Analogy

$v=0$ gravity ↓

$v=v_{max}$ elastic bar
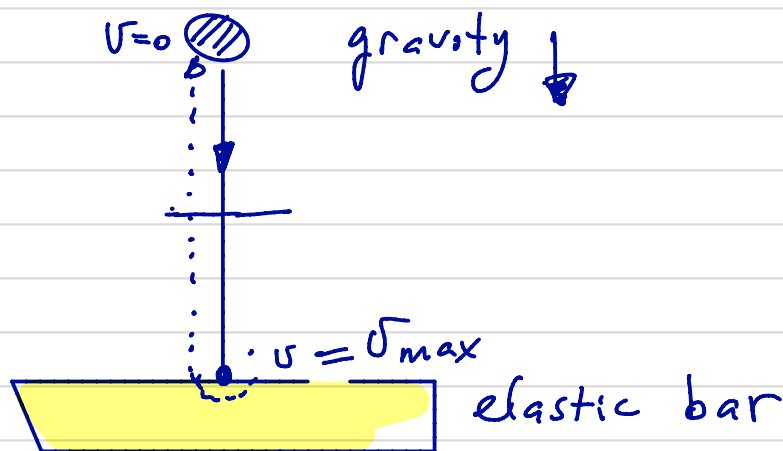
In other words by applying $-eE$ the electron experiences a periodic motion inside the crystal.

So oddly enough we can conclude that if we apply a constant $\bar{E}$ the electron moves <u>periodically</u> !

Lets determine it's frequency. The period of oscillations is determined by the time τ it takes to move from A to A'

From $\frac{\partial p}{\partial t} = e\bar{E}$ $\Rightarrow$ $\tau = \int_{-\pi\hbar/a}^{\pi\hbar/a} \frac{dp}{|e|E} = \frac{2\pi\hbar}{a|e||\bar{E}|}$

and $\nu_E = \frac{1}{\tau} = \frac{a|e||\bar{E}|}{2\pi\hbar}$

The Energy change $E_A - E_{\Pi}$ = work done by $|e|\bar{E}$ over X

$E_A - E_{\Pi} = e|E| X$ $\Rightarrow$

$X = \frac{E_A - E_{\Pi}}{2|e||E|}$ but recall

$E_A - E_{\Pi}$ is the BANDWIDTH!

$\sim$ few eVs.

and for $E \sim 10^{-6} \frac{V}{cm}$ $X \sim 10^6 cm$

and we could have observed those in the crystal, but for real crystals and for $T \neq 0 K$ we will have multiple scattering from phonons

and defects and the mean free path (mfp) $< 1 cm$! $<<$ X

This means that the reason we have conduction of electrons in a metal (as opposed to oscillations) is due to SCATTERING !

Q: WHAT WOULD HAVE HAPPENED IF WE HAD NO SCATTERING? AND WHY?
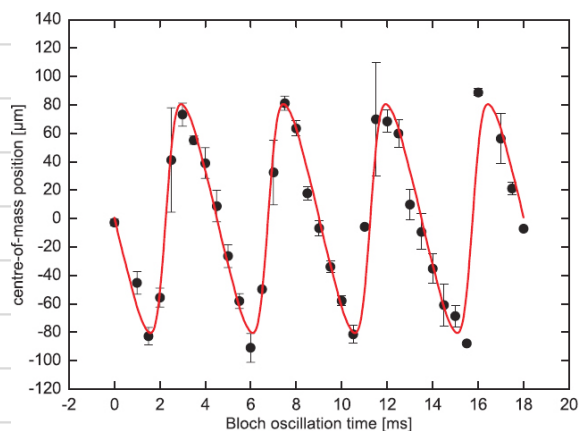
Bloch oscillations in a cold atom system (also see the wikipedia article about Bloch oscillations)

Mass of electron in solids

In classical mechanics "the real" mass is defined as

$$m_0 = F/a$$

In a crystal we have forces from ions which are not known in general.

But we can define the characteristic parameter called effective mass such as

$$m_0 \frac{dv}{dt} = \sum (F_{int} + F_{ext}) \implies m^* \frac{dv}{dt} = F_{ext}.$$

Lets compare it to the arb. dispersion eqn:

$$\frac{dv_i}{dt} = \frac{dv_i}{dp_k} \frac{dp_k}{dt}$$

So the ith component of the eqn. is

$$v_i = \frac{dE}{dp_i} \quad \text{and taking into account}$$

$$\frac{dp_k}{dt} = F_k \quad \text{we get} \quad \frac{dv_i}{dt} = \frac{\partial^2 E}{\partial p_k \partial p_i} F_k$$

$$\boxed{\frac{\partial^2 E}{\partial p_k \partial p_i} = \frac{1}{m^*_{ij}}}$$

m^*_{ij} is called the effective mass tensor.

Few notes:

1) Diagonal terms m^*_{ii} on the isoenergy surface are positive e.g. for a sphere

$$E = p^2/2m^* \Rightarrow m^* = \left(\partial^2 E / \partial p^2\right)^{-1} > 0$$

b/c $\frac{\partial E}{\partial p} > 0$ for electrons $\left(\frac{\partial E}{\partial p} = v < 0 \text{ for holes}\right)$

2) $\bar{a}$ the acceleration is not collinear with F

3) Different k_s for different positions on the Fermi surface correspond different m^* except for the extremal points.

4) The process of relaxation depends on how inelastic is the scattering

e.g. for many scattering events within τ the motion of electron or its phase has many resets. And as such one can think of it as a motion in the viscous enviroment.

The magnitude of the relaxation time defines the boundary when one can talk about quasiparticels: e.g. from
$\Delta E \cdot \tau \sim \hbar$ is possible to talk about the quasiparticens if $\Delta E \ll E_F$

if we have a very disordered enviroment or strongly correlated "Bad" metal where $\ell = v_F \cdot \tau \sim a$ (the so called Ioffe -Rögel limit)

$$\Delta E \sim \frac{\hbar}{\tau} = \frac{\hbar v_F}{\ell} = \frac{10^{-34} \, 10^6 \, J}{10^{-10}} = 10^{-18} \, J \sim 6 eV$$

Boltzmann equation and relaxation time

Boltzmann came up with a very general expression for all kinds of transport. This approach is standard in modern condensed matter physics since it describes the changes in the distribution function upon application of any perturbation.

* Relaxation time approximation:

Let's consider a single band and lets call $f(\bar{k}, t)$ the probability that a state with $\bar{k}$ occurs at time t. Normally it would be the Fermi-Dirac distribution in equilibrium, since $E(\bar{k})$

If the solid is not at equil. we have different f

$$\frac{df}{dt} = \left[\frac{\partial f}{\partial t}\right]_{field} + \left[\frac{\partial f}{\partial t}\right]_{scatt.}$$

$$\left[\frac{\partial f}{\partial t}\right]_{field} = \lim_{\Delta t \to 0} \frac{f(k, t+\Delta t) - f(k, t)}{\Delta t} \bigg/ _{field}$$

Note k remains unchanged.   Change in field during the time Δt.

e.g. in time Δt the state $\overset{k}{k} + \frac{eE}{\hbar} \cdot \Delta t \to$

$$f(k, t+\Delta t) = f(k + e\frac{E \Delta t}{\hbar}, t) = f(k, t)$$
$$+ eE \cdot \nabla_k f \, \Delta t / \hbar \to$$

$$\boxed{\left[\frac{\partial f}{\partial t}\right]_{field} = + \frac{eE \, \nabla_k f}{\hbar}}$$

As for the scattering rate we take very generally

$$\left[\frac{\partial f}{\partial t}\right]_{scatt} = - \frac{f(k,t) - f_0(k)}{\tau}$$

$\Rightarrow$ Fermi. Dirac distribution

$\leftarrow$ relaxation time

What we want is to understand how the tendency to equilibrium gets restored after we applied the field, e.g. $\bar{E}$. It's simple

If $f > f_0 \Rightarrow \left(\frac{\partial f}{\partial t}\right)_{scatt} > 0$ and $f \uparrow$.

Now suppose $f(k,0)$ $t=0$ is in non-equilibrium if $E = 0$ we get

$$\frac{\partial f}{\partial t} = - (f - f_0)/\tau \quad \text{(see prev. page)}$$

$$f(k,t) = f_0(k) + [f(k,0) - f_0(k)]e^{-t/\tau}$$

the distribution relaxes exponentially fast in time and for small τ it's almost in equilibrium.

Now we turn on the field:

$$\boxed{\frac{\partial f}{\partial t} = \frac{e}{\hbar} \bar{E} \cdot \nabla_k f - \frac{f - f_0}{\tau}}$$

The famous Boltzmann transport equation

Take $\quad f(\bar{k}, t) = f_0(\bar{k}) + f_1(\bar{k}, t)$

$\uparrow$ small deviation from equilibrium

$$\frac{\partial \left(f_0(k) + f_1(k,t) \right)}{\partial t} = \frac{e}{\hbar} E \cdot \nabla_k \left(f_0 + f_1 \right) -$$

$$- \frac{(f_0 + f_1) - f_0}{\tau}$$

$$\boxed{\frac{\partial f_1}{\partial t} = \frac{e}{\hbar} E \cdot \nabla_k f_0 - \frac{f_1}{\tau}} =$$

$$= e\bar{E} \cdot \vec{v} \frac{\partial f_0}{\partial E} - \frac{f_1}{\tau} \qquad \nabla_k f_0 = \frac{\partial f_0}{\partial E} \underbrace{\nabla_k E}_{= \hbar \bar{v}}$$
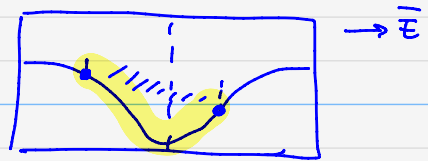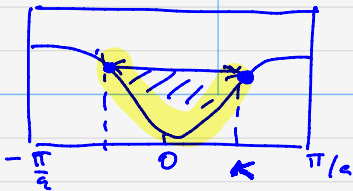
$t = 0$:   we turn on   the field and the solution is

$$f_1(k,t) = e E \cdot \vec{v} \tau \frac{\partial f_0}{\partial E} \left[1 - e^{-t/\tau} \right]$$

for $t \gg \tau$ the   electron   system   reaches the
steady   state:

$$f(k) = f_0(k) + f_1(k) = f_0(k) + e\bar{E} \cdot \vec{v}\tau \frac{\partial f_0}{\partial E}$$

Since $\frac{\partial f_0}{\partial E} < 0$

$-\frac{\pi}{a}$ 0 k π/a

$\rightarrow \bar{E}$

0

Lets now study what average momentum does

$$\hbar \bar{g} = \sum_{\hbar} \bar{g} f(\bar{g}, t)/N$$

going back to

$$\sum \hbar \bar{g} \times \left| \frac{\partial f}{\partial t} \right. = \left[\frac{\partial f}{\partial t} \right]_{field} + \left[\frac{\partial f}{\partial t} \right]_{scatt.}$$

over all
states in
the band

$$\frac{d \left(\hbar \bar{g} \right)}{dt} =$$

$$= \left(\frac{d \, \hbar \bar{g}}{dt} \right)_{field} \quad ?$$

for each electron

$$\frac{d \left(\hbar \bar{g} \right)}{dt} = -eE \quad \Rightarrow \quad \sum \frac{d \, \hbar g}{dt} = -eE,$$

momentum   over
                                        states

and if τ is independent of $\bar{k}$

$$\left(\frac{d \, \hbar \bar{g}}{dt} \right)_{scatt} = - \frac{\hbar \bar{g}}{\tau} \qquad \text{as the result}$$

we have

$$\frac{d \, \hbar \bar{g}}{dt} = -eE - \frac{\hbar g}{\tau}$$

and in the steady stat $t \gg \tau$

$$\hbar \bar{g} = -eE\tau \neq 0 \,!$$

unlike the case when electrons are at equilibrium

This means for metals only band crossing E_F
contribute to mobility μ.

Consider a hypotetical cubic xtal:

$$\mu_{ij} = \mu \quad \text{scalar}$$

for $i = j$ $v_i v_j$ and $-v_i v_j$ occur
equally so all those terms will cancel out

Also v_x^2, v_y^2, v_z^2 are the same $\Rightarrow$

$$\mu_{xx} = \mu_{yy} = \mu_{zz} \equiv \mu \Rightarrow$$

$$\bar{v} = -\mu E \quad \text{where} \quad \mu = \frac{1}{3}\left(\mu_{xx} + \mu_{yy} + \mu_{zz}\right)$$

$$\boxed{\mu^{e^-} = -\frac{e}{3N} \sum \tau v^2 \frac{\partial f_0}{\partial E}^{\text{electrons}}}$$

Since $\frac{\partial f_0}{\partial E} < 0 \Rightarrow \mu > 0$ for electrons, but $\bar{v} \uparrow \downarrow \bar{E}$

For non-cubic xtals it's also ok but

$$\tau = \tau(\bar{k})$$

Similarly for hole we can write down

$$\boxed{\mu^{\text{holes}} = \frac{e}{3N} \sum \tau v^2 \frac{\partial f_0}{\partial E}^{\text{holes}}}$$

$$\frac{\partial f_0^{\text{holes}}}{\partial E} > 0 \quad \text{and} \quad \mu > 0 \quad \text{but} \quad \bar{v} \parallel \bar{E}$$

Physical meaning of $\bar{g}$:

suppose at $t=0$ $g=0$ then for the time τ it accelerates and becomes $-eE\tau$ but returns back to $g=0$ after scattering. That's why $\underline{\tau}$ is $\underline{\text{mean free time}}$.

$\underline{\text{Mobility}}$: In the steady state $\bar{v} \sim E$ ...average velocity
and thus:

$$\bar{v}_i = -\sum_j \mu_{ij} E_j \quad \leftarrow \text{mobility}$$

often called electron drift velocity

Lets try to obtain the expression for μ_{ij}

1. Start with

$$\bar{v}_i = \frac{1}{N} \sum_{\text{states}} v_i(k) f(k)$$

# of electron in the band

and $f(k) = f_0(k) + eE \cdot \bar{v}\tau \frac{\partial f_0}{\partial E}$

$$= \frac{1}{N} \sum \underbrace{v_i(k) f_0(k)}_{=0} + \frac{1}{N} \sum v_i \, eE\bar{v}\tau \frac{\partial f_0}{\partial E}$$

$$= \frac{e}{N} \sum_{\text{states}} v_i \, \bar{E} \cdot \bar{v} \, \tau \frac{\partial f_0}{\partial E} \implies$$

$$\mu_{ij} = -\frac{e}{N} \sum_{\text{states}} \tau \, v_i v_j \frac{\partial f_0}{\partial E}$$

Since $\frac{\partial f_0}{\partial E}$ spikes only at E_F only the state at the chem. potential matter.

Electrical Conduction in bands

$$\bar{J} = q \, n \, \bar{v} \quad \text{in } E\&M$$

In solid state physics:

the carrier density $\quad n = \dfrac{f(\bar{k})}{V}$

$$\bar{J} = -\frac{e}{V} \sum_{\text{states}} f(\bar{k}) \, \bar{v}(\bar{k})$$

Sum over states can be done like 1-band at the time and $\sum f(\bar{k}) \bar{v}(\bar{k})$ over states in the band can be identified as $N \cdot \bar{v}$

$N = \#$ of e^- in the band, $\bar{v}$ — average velocity

So:
$$\dot{J} = -e \sum_{\text{bands}} \frac{N}{V} \cdot \bar{v} = -e \sum_{\text{bands}} n \, \bar{v}$$

where n is the contribution of the band to total electron concentration.

Recall for the steady state $\bar{v}_i = -\sum_j \mu_{ij} E_j$

$$\boxed{\dot{J}_i = e \sum_{\text{bands}} \left[n \sum_j \mu_{ij} E_j \right]} \quad \text{and}$$

remembering Ohm's law $\quad J = \sigma E \implies$

$$\dot{J}_i = \sum_j \sigma_{ij} E_j \quad \text{where}$$

$$\boxed{\sigma_{ij} = e \sum_{\text{bands}} n \, \mu_{ij}} \quad \begin{array}{l}\text{the conductivity}\\ \text{tensor}\end{array}$$

WITH THIS INFO LETS LEARN ABOUT
ELECTRON — PHONON SCATTERING

1. Quasi momentum of e^- doesn't change when it moves in an ideal periodic lattice

2. It can change only interactions with NON periodic part of the potential.

   e.g. phonons, defects, dislocations, domain boundaries surface, interface, grain boundaries

   AND $e - e$ interaction   or $e-e$ scattering

3. we have inelastic and elastic processes.

Now to the phonons: phonon is an elastic phase of deformation as the result we have an additional periodicity to the potential on which electrons can scatter off.

The effect is connected to the # phonons the electron can scatter.

Note: Similar to the phonon story during the scattering act we should consider both N-process and U-process

   ↑ no crystal   ↑ with crystal
     momentum   momentum.

But unlike phonons which has no chemical potential and thus no Fermi surface.
Electrons scattering is strongly bound to the topology of Fermi surface.

Electrical conductivity

Basics: in absence of ∇T and diffusion

$$\bar{J} = \sigma \bar{E}$$

↑ electrical conductivity

In isotropic cas $\bar{J} \parallel \bar{E}$ and σ is a scaler
But we know that almost all real crystals
have anisotropy of some sort, in this case:

$$j_i = \sum_k \sigma_{ik} E_k \quad , \quad \Rightarrow \quad E_i = \sum_k \rho_{ik} j_k$$

↑ tensor!

↑ resistance tensor

the connection $\sigma_{ik} \rho_{ik} = \delta_{ik}$
also $\rho_{ik} = \rho_{ki}$

The components can be determined by measuring
electric field along crystal axis 1, 2, 3

along 1: e.g $\quad E_1 = \rho_{11} j_1 \quad E_2 = \rho_{21} j_1$ etc

along 2: $\quad\quad E_1 = \rho_{12} j_2 \quad E_2 = \rho_{22} j_2$ etc

In cubic x[al] all non diagonal terms = 0
for a single axis materials:

$$\rho_{11} = \rho_{22} \neq \rho_{33}$$

Electrical conductivity in the model of Fermi carriers

– Lets assume we deal only with close FS
– and the only scatterers are _phonons_.
– Also lets assume the FS is close to spherical e.g. K, Li
 Na...

$E(p) = \frac{p^2}{2m^*}$, τ – time between scattering

$W_{k,k'}$ is the probability of scattering from $k \to k'$

$W_{k,k'} \sim \frac{1}{\tau}$. After that the electron moves

$\ell = v_F \cdot \tau$.
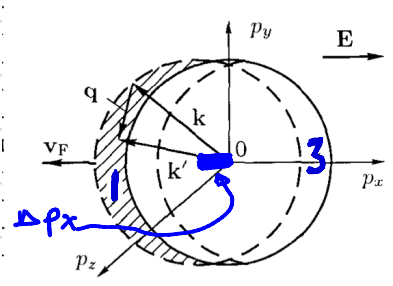
Apply E along x.
All electrons get extra $\Delta p_x = -e E_x \tau$

The whole distribution moves in the opposite direction by Δp_x.

Without $\bar{E}$ we have no j since
for each e^- with $+\bar{p}$ we have e^- with $-\bar{p}$
With application of E central symmetry is broken.
Now we have uncompensated charge in ① and ③

On the FS for electron we have $m^* > 0$
and $v_F \perp$ to the FS. Electrons in 1 and 3
create a flow of electrons with $v \sim v_F$ along $\bar{F} = -e\bar{E}$
+ The higher $\bar{E}$ the large the volume.

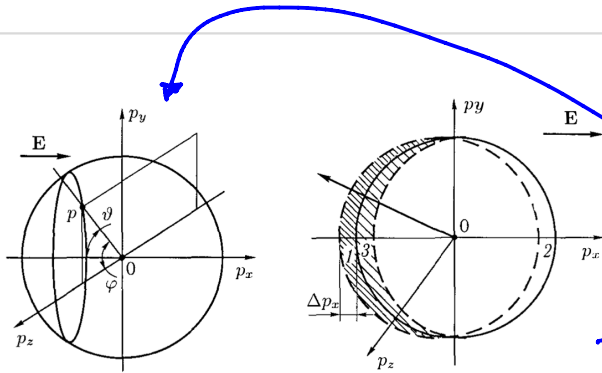Now consider holes: For hole $\frac{d\bar{p}}{dt} = -e\bar{E}$
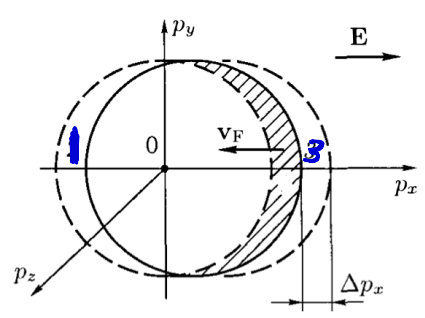
In volume ① we have e^-
② we deplete electrons

As the result, e^- with $v \sim v_F$
in ① and ③ create current
in the same direction as electrons

As the result in metals with electrons and holes, current
is a sum of e^- and h.

Electrical Conductivity

To derive the equation for σ, consider the spherical coordinates. Since $\Delta p \ll p_F$ any particle in 1 and 3 is along p and $v \sim v_F$. The projection of v onto $-\bar{E}$ is $p\cos\vartheta / m^*$, since velocities ① and ③ are practically identical, we calculate the current in ①

— inside $dv_p = p^2 \sin\vartheta \, dp \, d\vartheta \, d\varphi$ we have

$$\Delta n = \int \frac{dv_p}{(2\pi\hbar)^3} \text{ electrons}$$

spin ↑ and ↓

The contribution of those electrons into current

$$dj = e \Delta n v = e \frac{2 p^2 \sin\vartheta \, dp \, d\vartheta \, d\varphi}{(2\pi\hbar)^3} v_F \cos\vartheta$$

The total current created by e^- in the volumes 1 and 3 thus:

$$j = 2 \cdot \frac{2e v_F}{(2\pi\hbar)^3} \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\varphi \int_{p_F}^{p_F + \Delta p \cos\vartheta} p^2 \sin\vartheta \cos\vartheta \, dp =$$

$$= \boxed{j = \frac{8\pi e \, p_F \, v_F \, \Delta p_x}{3 \, (2\pi\hbar)^3}}$$

Show this

$4\pi p_F^2 = $ the area of the isoenergy surface for e^- and since $\Delta p_x = e E \tau = e \cdot \ell_m E / p_F$

$$j = \frac{2}{3} \frac{e^2 S_F \ell}{(2\pi\hbar)^3} E$$

and from $j = \sigma E \Rightarrow$

$$\sigma = \frac{2}{3} \frac{e^2 S_F \ell}{(2\pi\hbar)^3}$$

this eqn. is known as the Lifshits eqn.

It works for any dispersion as long as

$E(p) = f(p^2)$ and f has no singularities.

Lets consider the simplest case $E = p^2/2m^*$
(BTW the linear dispersion is also can be of this kind, i.g. $E^{\pm} = \pm \alpha (p^2)^{1/2}$!) for whic $p = 0$ is a singularity.

Lets rewrite eqn for σ as:

$$S_F = 3\frac{D_F}{p_F} \Leftarrow (\text{indeed } S_F = 4\pi p_F^2 \text{ and}$$

the volume in momentum space

$$D_F = \frac{4}{3}\pi p_F^3)$$

Also recal for isotropic dispersion
$$p_F = m^* v_F$$

we get $\sigma = \dfrac{2e^2 D_F \ell}{(2\pi\hbar)^3 m^* v_F} = \dfrac{e\tau}{m^*} \dfrac{2D_F}{(2\pi\hbar)^3}$

↑ this is concentration of e^- thus we can write down

$$\sigma = \frac{e^2 n \tau}{m^*}$$

Which is exactly the famous formula
$$\sigma = en\mu \quad \text{known as Drude formula.}$$
clearly $\dfrac{e^2 n \tau}{m^*} = en\mu \Rightarrow \boxed{\mu = \dfrac{e\tau}{m^*}}$ Mobility

14

!!!

a — ZnO

2009: Optimization of growth rate
2008: Molecular-beam epitaxy
2007: Pulsed-laser deposition
Bulk mobility

b — 2D mobility in GaAs
2007: MBE growth conditions
2000: Sample structure
1988: UHV cryopumpbake   36 million cm² V⁻¹s⁻¹
1986: As, Al, Ga source purity
1982: LN2 shielded sources
1981: Sample loadlock
1980: Single interface
1979: Undoped setback
1978: Modulation doping
Bulk mobility at these carrier densities

Ignore This! → **Electrical conductivity in the electron-hole model**

Resistivity (nΩ m)
Inconel-825
NiCr heating wire
Monel-400   Platinum   Tungsten
Iron
Nickel   Aluminum / Gold / Copper / Silver
$p \propto T$
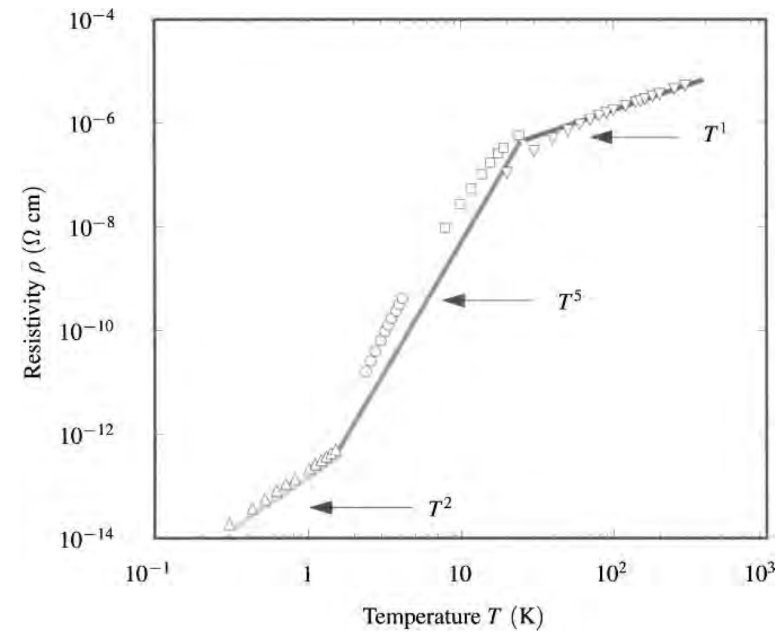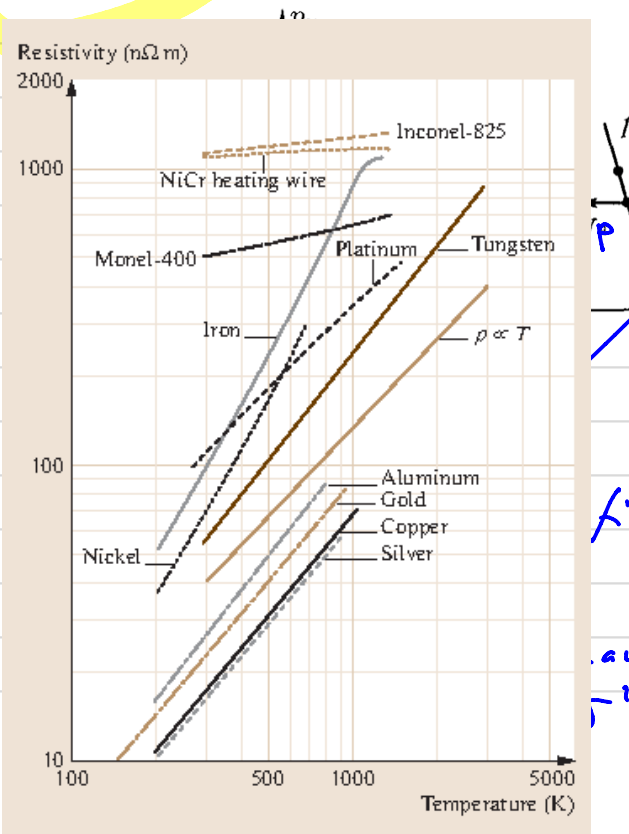
Figure 18.1. Resistivity of potassium from 0.1 to 300 K. At the lowest temperatures, the resistance varies as T^2, from 2 to 20 K, it varies as T^5, and from 100 K upwards, it varies as T^1. [Source: Bass et al. (1990).]

TEMPERATURE DEPENDENCE OF CONDUCTIVITY

Clearly the T-dep. comes from the T-dependent $\tau(T)$
In this theory we consider that the only important
processes are those when $\Delta p \sim p$ or the electrons
is transfered from ① in ② and as such
we need the <u>U-process.</u>

The time which takes for the e^- to move
from ① → ② is called the <u>transport relaxation
time.</u>

When $T > T_D$ e^- and phonons have momentum
which $\sim \frac{\pi}{a} \cdot \hbar$. The # of phonons for $T > T_D$
$\overset{\text{scattering}}{}$

$T > T_D$ $\Big|$ $\sim T$, thus $\tau_t \sim \frac{1}{T}$ and $\sigma \sim \tau_t \sim \frac{1}{T}$
and $\rho \sim T$

But when the momentum of phonons is small $T \ll T_D$
we have a problem to move from ① → ②.
which now can only happen as the result
of <u>diffusive motion.</u> (see fig. on p. 11)
$k \to k'$

As the result for each scattering act
e^- with $\vec{p}$ with phonon with $\vec{q}$
the projection of of e^- momentum on to the
direction of initial motion is:

$\Delta p = p(1 - \cos\alpha)$
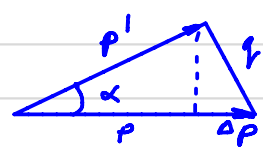
$\Delta p = (1-\cos\alpha)p$
$\cos\alpha \sim 1 - \alpha^2/2$
$\alpha = q/p$

So we get $\Delta p = p(1-\cos\alpha) = \frac{\alpha^2 p}{2} \propto \frac{q^2}{2p}$

Recall that $p \sim \hbar \frac{\hbar}{a}$, and the momentum of phonons is
given by $\hbar\omega_{ph} = v_a q \ll k_B T \Rightarrow q \cong k_B T / v_a$

and also recal that $T_D \sim \frac{\hbar \omega^{max}}{k_B}$

for ω^{max} we have $\lambda_{min} \simeq 2a \implies$

$$T_D \approx \frac{\hbar \omega^{max}}{k_B} = \frac{2\pi \hbar \sigma_a}{2a \, k_B} \propto \frac{\sigma_a \, p}{k_B}$$

and as the result we have

$$\Delta p \approx \frac{q^2}{2p} = \frac{k_B^2 \, T^2 \, \sigma_a^2 \, p}{2 \, \sigma_a^2 \, k_B^2 \, T_D^2} \simeq \left(\frac{T}{T_D}\right)^2 p$$

To scatter e^- we must turn in into the angle $\pi/2$ and the projection of the $\Delta p \sim p_F \implies$

The number of acts like this $\underset{\substack{\text{Scales} \\ \text{with}}}{\frac{p}{\Delta p}} \sim \left(\frac{T}{T_D}\right)^2 \sim \frac{1}{T^2}$

The number of available phonons for $T \ll T_D \sim T^3$

$T \ll T_D$: Thus for the scattering of e^- on phonons with $\omega \ll \omega^{max}$

$$\tau_t \sim \left(\frac{1}{T^2}\right) \cdot \left(\frac{1}{T^3}\right) \implies \boxed{\begin{array}{l} \sigma \sim \frac{1}{T^5} \\ \text{and} \quad \rho \sim T^5 \end{array}}$$

For the case of spherical FS and very specific spherical distribution of phonon momentum there is a general formula called the

Bloch – Grüneisen formula.

$$\rho_{el-ph} = \alpha_{el-ph} \left(\frac{T}{\theta}\right)^n \int_0^{\theta/T} \frac{x^n}{(e^x - 1)(1 - e^{-x})} \, dx, \qquad \overset{\equiv \theta_D}{\nearrow}$$

U - process in ē-phonon scattering

$\hbar\omega = \hbar\omega_q$

BZ

E_{Fermi}

$E_k = E_F$ $E_{k'} = E_k + \hbar\omega_q$ Q

N_s = Concentration of scatters

$\ell = u\tau$ Scatterer S
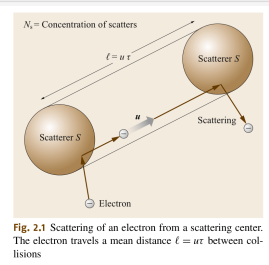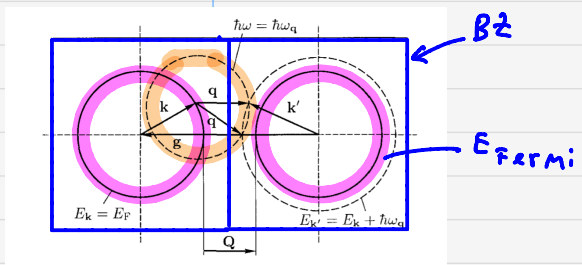
Scatterer S Scattering

Electron

Fig. 2.1 Scattering of an electron from a scattering center. The electron travels a mean distance $\ell = u\tau$ between collisions
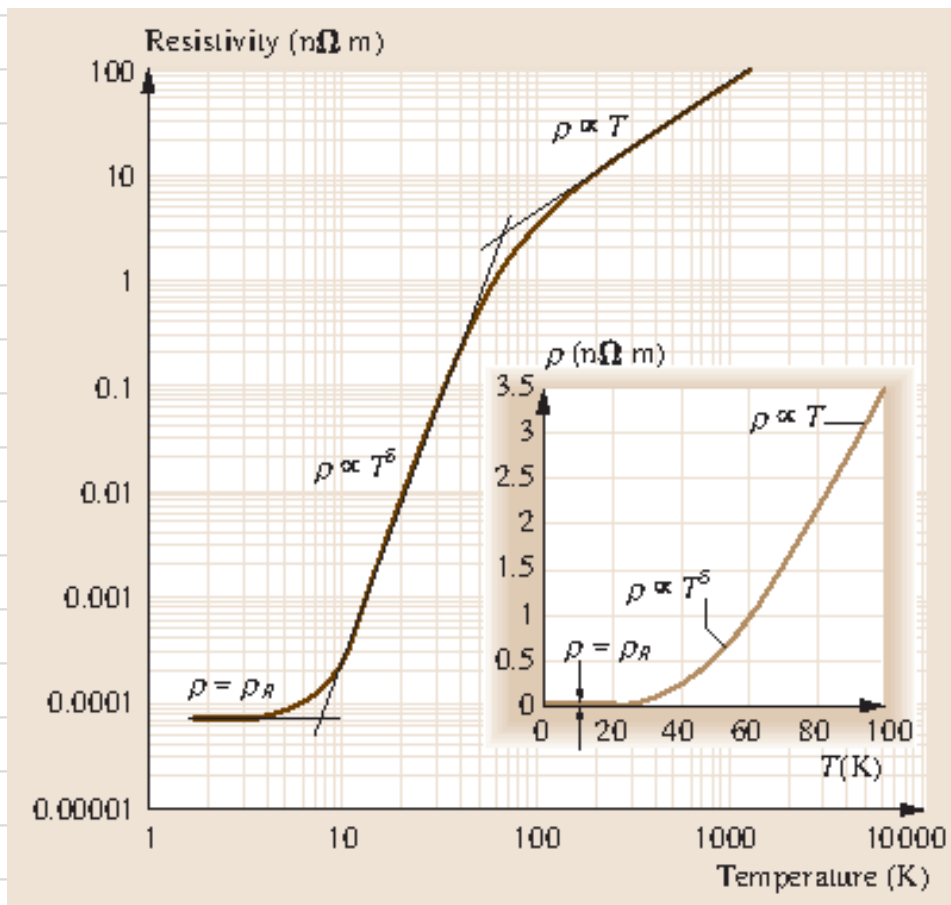
Here we have: $E(k') = E(k) + \hbar\nu_q$
and $\hbar k' = \hbar k + \hbar q + \hbar g$
                          ↳ xtal momentum

What's important, for a given k
there will be a specific phonon with q, such
that $w(q) = E(k') = E(k) + \hbar w$
            ↗   ↳ isoenergy surface

But unlike N-process the intersection will
disappear at some $|q| = Q$.
The closer E_F's in the neighboring BZ are
the more important is U-process.
    e.g. in alkali metals U-process is
dominant event at $T = 20k$!

The resistivity of copper from low to high temperatures (near its melting temperature, 1358K) on a log–log plot. Above about 100K, $\rho \propto T$, whereas at low temperatures, $\rho \propto T5$, and at the lowest temperatures ρ approaches the residual resistivity ρR. The inset shows the ρ versus T behavior below 100K on a linear plot. (ρR is too small to see on this scale.)
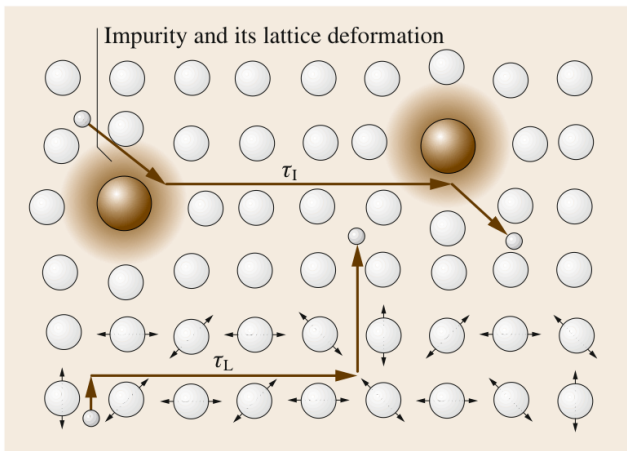
Matthiessen rules

Impurity and its lattice deformation

Fig. 2.3 Scattering from lattice vibrations alone with a mean scattering time τ_L, and from impurities alone with a mean scattering time τ_I

Experiment shows
that the following is correct:

if different independent

microscopic processes
underlie the collisions of
electrons at the Fermi surface
the probalities of the
collisios are [additive]

SPECTRAL DENSITY OF STATES
FOR e⁻

Distribution of e⁻ states by energy is one of the most important things to characterize the electronic spectrum excitations.

Lets introduce an important parameter THE **DENSITY OF STATES**.

if $N(E)$ is the # of states with energy $\leq E$ $\Rightarrow$

$dN(E)$ is the # of states between E and $E + dE$

Spectral density of states $\nu(E)$ (sometimes $g(E)$ or $D(E)$)

$$= \underbrace{\frac{dN(E)}{dV}}_{dn(E)} / dE = \frac{dn(E)}{dE}$$

clearly we have a connection to $E(p)$

e.g. recal for free electrons

$$n \overset{3D}{=} \frac{2 m_0 E_F(0)]^{3/2}}{3 \pi^2 \hbar^3} \Rightarrow$$

$$\mathcal{D} \overset{3D}{=} \frac{dn}{dE} = \frac{(2m_0)^{3/2} \sqrt{E_F(0)}}{2 \pi^2 \hbar^3} = \frac{\sqrt{2} \, m_0^{3/2} \sqrt{E_F(0)}}{\pi^2 \hbar^3}$$

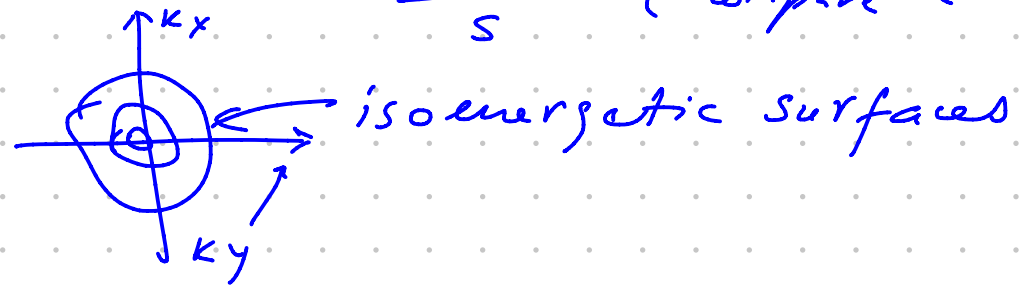$\Rightarrow$ the carrier density $n = \int_0^{E_F(0)} \frac{dN}{dE} dE =$

$\Rightarrow$ For finite T, we need to include
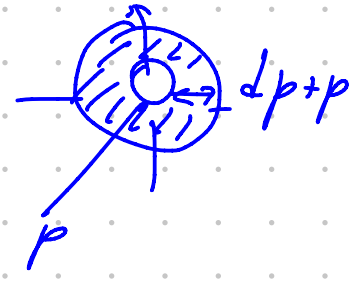
$$n = \int_0^{\infty} f E_n \frac{dn}{dE} dE$$

Lets derive the expression for 2D

For 1 state the area is $\frac{(2\pi\hbar)^2}{S}$ (compare $(2\pi\hbar)^3/V$)

For $E = \frac{p^2}{2m^*}$ — isoenergetic surfaces

The # of states

$$dN_p^{2D} = \frac{4\pi(p+dp)^2 - 4\pi p^2}{(2\pi\hbar)^2}$$

$$= \frac{4\pi S p \, dp}{(2\pi\hbar)^2}$$

and b/c $dE = \frac{p \, dp}{2m^*} \Rightarrow$

$dp = \frac{m^*}{p} dE$

$p \, dp = m^* dE$

$\Rightarrow dN_p^{2D} = \frac{4\pi S m^* dE}{(2\pi\hbar)^2} =$

$= \frac{4\pi m^* dE}{(2\pi\hbar)^2}$

$$\boxed{\nu^{2D}(E) = \frac{m^*}{\pi\hbar^2}}$$

! it's independent of Energy for 2D and is defined only by the effective mass of m^* (of course for parabolic $E = p^2/2m^*$)

In general however m^* depends on E
$\Rightarrow \nu^{2E}$ also depends on E

Q₁: Show for anisotropic $E = P_x^2/2m_x + P_y^2/2m_y$

$$\nu^{2D}(E) = \frac{\sqrt{m_x m_y}}{\pi\hbar^2}$$

Q₂: Show that for 1D:

$$\nu^{1D}(E) = \frac{L\sqrt{m^*}}{\sqrt{2}\,\pi\hbar\sqrt{E}}$$

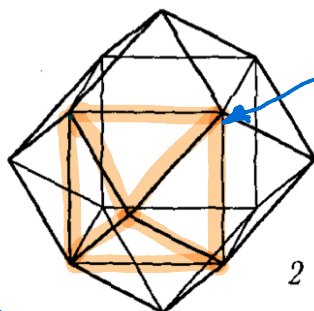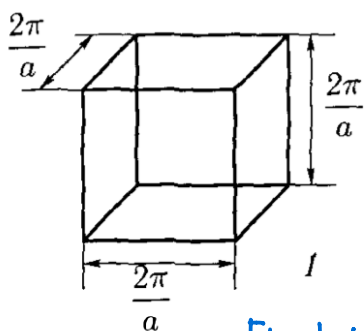L is the length of the xtal.

Van Hove singularities:

It is clear that to calculate $\nu(E)$ one **22**
needs to know $E(\vec{p})$. However we can try
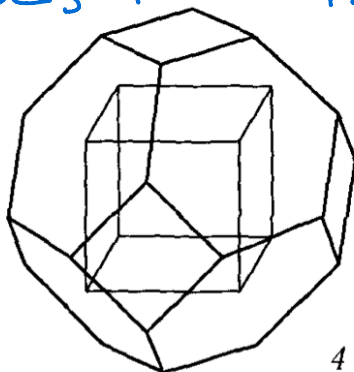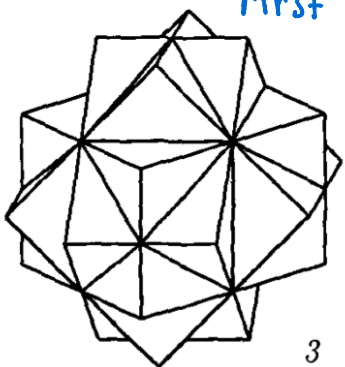to get an idea what happens when we fill up the BZ.
Consider a square lattice with a period a:

 $\Rightarrow$ $\frac{2\pi}{a}$ $2\pi/a$

As seen 2^d BZ is made of 6 pyramides built on on the faces of the 1st BZ
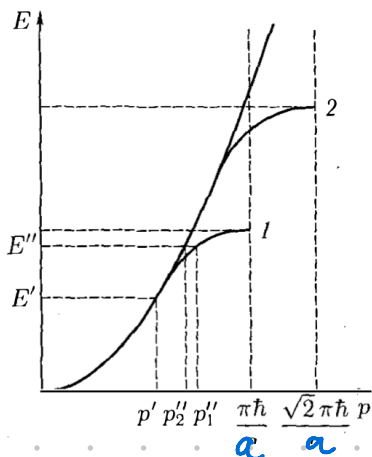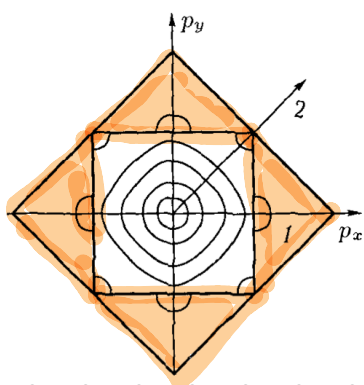

First 4 BZs for cubic lattice

The min of energy is at $\sigma=0$ for 1st BZ

The dispersion $p^2/2m^*$ and $\nu^{3D}(E) \sim \sqrt{E}$

Note for $E=0$
$$\frac{d\nu}{dE} \nearrow \infty$$

With increasing E the sphere gets distorted when it approaches the 2D BZ

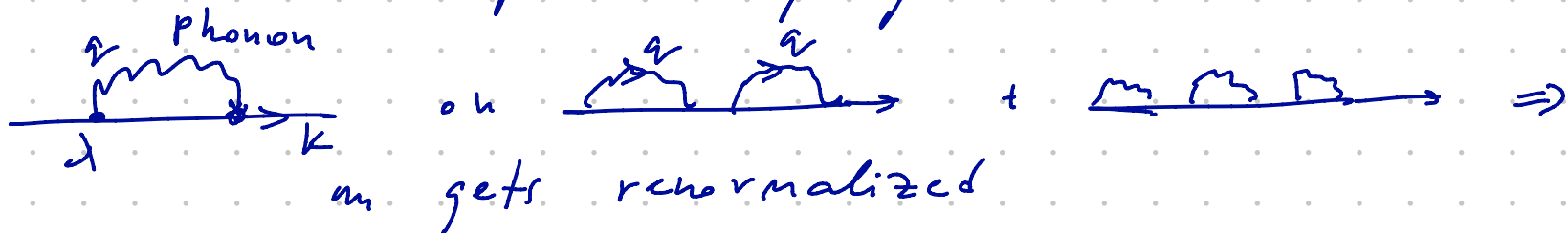## Renormalization of density of states due to electron-phonon coupling.

The polarization of lattice leads to the fact that

m_{ij}^* is different from $\dfrac{1}{\frac{\partial^2 E}{\partial k_j \partial k_j}}$

and often can be written as $m^* = m_{band}(1+\lambda)$

$\lambda =$ electron-phonon coupling

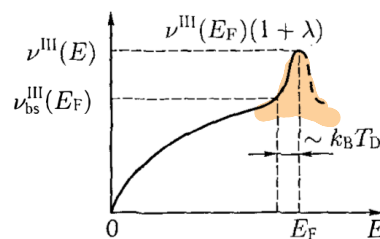m gets renormalized

Since $m \uparrow \Rightarrow \mathcal{D}(E)$ goes up near the Fermi surface within $k_B T_D$; since $\mathcal{D}^{3D}(E) \sim (m_s^*)^{3/2} \Rightarrow$

$$\mathcal{D}^{3D}(E) = (1+\lambda)^{3/2} \mathcal{V}_{band}(E) \Rightarrow$$

near E_F we get a peak

λ	Na	Al	Pb
	0.2	0.4	1.6

— Also e-ph coupling reduces E_F since $E_F \sim \dfrac{1}{m^*}$

Second we know for $T=0k$ $n = \displaystyle\int_0^{E_F} \mathcal{V}^{3D}(E)\, dE$

if $\mathcal{V}^{3D} \uparrow$ E_F must go down

— Also λ doesn't affect the size of F.S. as it only depends on $\underline{\underline{n}}$ and the lattice geometry.

— B/c of λ since $\mathcal{D}^{3D}(E) \uparrow$ within $k_B T_D$ the fermi velocity goes down by $(1+\lambda)^{3/2}$.

Proof: $|v| = \dfrac{\partial E}{\partial p} = \dfrac{\partial E}{\partial N}\dfrac{\partial N}{\partial p} \Rightarrow v = \dfrac{\partial N}{\partial p}\cdot \dfrac{1}{\mathcal{D}(E)} \approx \dfrac{1}{(1+\lambda)^{3/2}}$

Electronic heat capacity and thermal Conductivity

The energy of quasi particles is given

$$E = 2 \cdot \frac{2V}{(2\pi\hbar)^3} \overset{\uparrow\downarrow \, spin}{\int_{p_F}^{\infty}} E(p) f_{E_n} \, 4\pi p^2 dp$$

two branches
one for electrons
and another for holes.

electronic heat capacity =

$$= \frac{1}{V}\left(\frac{\partial E}{\partial T}\right)_V = 4\int_{p_F}^{\infty} E(p) \frac{\partial f_n}{\partial T} \frac{4\pi p^2 dp}{(2\pi\hbar)^3}$$

using $\nu^{3D}(E) = \frac{\sqrt{2} \, m^{*3/2} \sqrt{E}}{\pi^2 \hbar^3}$, for isotropic model

$$\nu^{3D}(\epsilon_F) = p_F m^* / \pi^2 \hbar^3$$

$\color{red}{Q: \text{ Show that } \frac{1}{V}\left(\frac{\partial E}{\partial T}\right)_V = \int \cdots = \frac{\pi^2}{3} k_B^2 \, \nu^{3D}(\epsilon_F) T}$

and using $\nu^{3D}(\epsilon_F) \Rightarrow$

$$\boxed{C_e = \frac{p_F \, m^*}{3\hbar^3} k_B^2 T}$$

Thus we get $C_e(T) \sim T$ by measuring

C_e we can estimate $\dfrac{p_F \, m^*}{3\hbar^3}$ or m^*

In fact this is the most popular method for
geting m^* in crystals.

— Note E is the sum of all excitations. Consider
The averge energy of one excitation $\sim k_B T$
and their # scales with the with of $d\epsilon_F \sim k_B T$
Since $\epsilon_F = p_F^2 / 2m^* \rightarrow d\epsilon_F = p_F dp_F / m^* \rightarrow dp_F = m^* d\epsilon_F / p_F$
$$\approx m^* k_B T / p_F$$

The total energy of elementary excitation
inside dE is $E \sim N k_B T$

and the # of states is

see bottom of 24

$$N = \frac{4\pi P_F^2 \, \boxed{dP_F}}{(2\pi \hbar)^3} \approx \frac{4\pi P_F^2}{(2\pi \hbar)^3} \frac{m^* k_B T}{P_F}$$

and thus the energy $E \sim N k_B T = \frac{4\pi P_F \, m^* k_B^2 T^2}{(2\pi \hbar)^3}$

$$\Rightarrow \quad c_e = \frac{\partial E}{\partial T} \sim \frac{8\pi P_F k_B^2 m^* T}{(2\pi \hbar)^3} = \boxed{\frac{P_F \, m^* \, k_B^2 T}{\pi^2 \hbar^3}}$$

for $k_B T \ll E_F$

Lets compare it to the Debye expression for c_e

$$C_{Debye}^{3D} = \frac{12\pi^4 k_B N}{5} \left(\frac{T}{T_D}\right) \approx 234 \, k_B \, N \left(\frac{T}{T_D}\right)^3$$

$$\frac{P_F \, m^* \, k_B^2 T}{\pi^2 \hbar^3} \quad \longleftrightarrow \quad 234 \, k_B \, N \, \frac{T^3}{T_D^3} \quad \Rightarrow$$

$$C_{Debye}^{3D} = C_e \quad \text{at} \quad T' \sim 0.145 \sqrt{\frac{k_B T_D}{E_F}} \, T_D$$

meaning that if $T < T'$ the main contribution comes
from __electrons__! Lets estimate when it happens

$$E_F = \frac{P_F^2}{2m_0} \sim \frac{1}{2m_0} \left(\frac{\pi \hbar}{a}\right)^2 \quad \text{and} \quad \theta_{Debye} \sim \frac{2\pi v_a}{a}$$

with $v_a \sim 10^5 \, cm/s$ and $a = 10^{-8} \, cm$ $\quad T'/T_D \sim 3 \cdot 10^{-3}$

and $T \sim 0.5 K$. Which means that C_e

dominates at $T \sim T_{L \, Helium}$.

TC in metals is made of γ_{e^-} and $\gamma_{phonons}$

so $\gamma = \gamma_e + \gamma_{ph}$

As for electric conductivity $\overset{\text{heat resistance}}{\longrightarrow} W_e = \frac{1}{\gamma_e}$ and in general

$W_e = \sum_i W_{ei}$. Notice under thermal scattering

we assume such processes when after interaction
the quasiparticle <u>loses a portion of heat energy $\sim k_B T$</u>
but gets <u>extra momentum</u> due to <u>heat gradient</u>

Every act like this is characterized by τ_i and

$\ell_i = \sigma_g \tau_i$

and like for electricity $1/\tau_e = \sum_i \left(\frac{1}{\tau_e}\right)_i$

Lets assume a gas model:

$$\gamma_e = \frac{1}{3} C_e v \ell \qquad \ell = \sigma \tau \Rightarrow$$

$$\gamma_e = \frac{1}{3} C_e \sigma^2 \tau$$

As shown on p.25 $C_e \sim T$ and $\sigma \sim v_F \Rightarrow$

$$W_e = \frac{1}{\gamma_e} \sim \frac{1}{T v_F^2 \tau} = \frac{1}{T v_F^2}\left(\frac{1}{\tau_{e-ph}} + \right.$$

$$+ \frac{1}{\tau_{e-defect}} + \frac{1}{\tau_{e-e}}\left.\right) = \frac{1}{T v_F^2}\left(\nu_{e-p} + \nu_{e-d} + \nu_{e-e}\right)$$

Notice for thermal conductivity charge plays no role
so for the 1st approx. holes and electrons are the same.
Since the average energy of quasiparticles $k_B T$
the single scattering may lead to exchange $\sim k_B T$

This means that the probability of scattering on phonons is largely defined by the # of phonons.

For good crystals, the number of ph. is always $\gg$ defects, and the last term is usually $\ll \frac{1}{\tau_{e-p}}$ and $\frac{1}{\tau_{e-b}}$

So for high enough $T \geqslant T_D$

$$W_c \sim \frac{\nu_{e-p}^N + \nu_{e-p}^U}{T U_F^2}$$

for $T > T_D$ the # of phonons $\sim T$ and thus

$$\underline{W_c \text{ is independent of } T!}$$
$$T \geqslant T_D$$

for $T \ll T_D$ $\nu_{e-p}^N \sim T^3$ and the number of scatterings is determined by the # of phonons with $q > Q$

$$\nu_{e-p}^U \sim e^{-\frac{U_a Q}{k_B T}}$$

$\hbar\omega = \hbar\omega_q$

$E_k = E_F$ $E_{k'} = E_k + \hbar\omega_q$

$\Downarrow$

$$W_e \sim \frac{1}{T U_F^2}\left(\alpha T^3 + \beta e^{-\frac{U_a Q}{k_B T}}\right)$$

$$\sim \frac{1}{U_F^2}\left(\alpha T^2 + \frac{1}{T}\beta e^{-U_a Q/k_B T}\right)$$
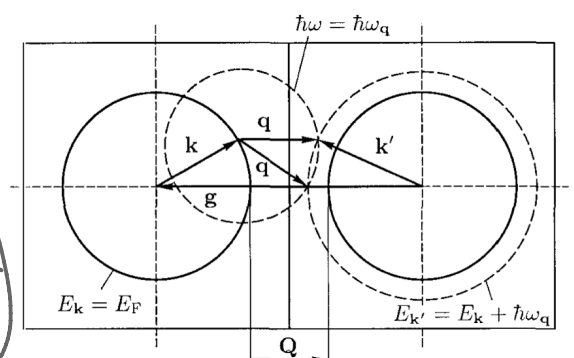
In the area where we can neglect U processes compared to N we get

$$W_e \sim T^2 \quad \text{and} \quad \gamma_e \sim T^{-2}. \text{ For very low } T$$
$$\nu_{e-def} \gg \nu_{e-p}$$

and ℓ_e, τ_e and ν_e become T-independent. Thus we get in this area $\gamma_e \sim T \to$ (all terms inside the bracket T-inde- -pendent)

γ_e

$\sim T$ $\sim T^{-2}$

const

0 θ_D T