I. Discussion on Scattering

$$\left(\frac{\partial f(\vec{r},\vec{k},t)}{\partial t}\right)_{\text{scattering}} = -\frac{(f-f^0)}{\tau} \equiv -\frac{g}{\tau} \qquad (50)$$

scattering-induced time evolution of $f(\vec{r},\vec{k},t)$ [or $f(\vec{k},t)$ in uniform $\vec{\mathcal{E}}$-field]

- Scattering processes: change electron state from $\vec{k}$ to $\vec{k}'$ ($f(\vec{k})$ drops)
  and from $\vec{k}'$ to $\vec{k}$ ($f(\vec{k})$ increases)

Let $W(\vec{k},\vec{k}')$ = rate of scattering from state $\vec{k}$ to $\vec{k}'$ ($\frac{1}{\text{time}}$ quantity)
(needs state $\vec{k}$ is occupied and state $\vec{k}'$ is empty)

$$\left(\frac{\partial f(\vec{k})}{\partial t}\right)_{\text{scattering}} = \int \left[f(\vec{k}')(1-f(\vec{k}))\underbrace{W(\vec{k}',\vec{k})}_{\text{into } \vec{k}} - f(\vec{k})(1-f(\vec{k}'))\underbrace{W(\vec{k},\vec{k}')}_{\text{out of } \vec{k}} \right] \underbrace{\frac{d^3k'}{(2\pi)^3}}_{\text{from all possible } \vec{k}'} \cdot V \qquad (51)$$

- This is the formal expression of $\left(\frac{\partial f}{\partial t}\right)_{scattering}$
- $W(\vec{k},\vec{k}')$ is a quantity for quantum mechanical calculations
- The relaxation time approximation puts the complexity into $\frac{1}{\tau(\vec{k})}$

General Aspect of Elastic Collisions

- energy unchanged e.g. impurity scattering / alloy scattering $Ga_{1-x}Al_xAs$

$$W(\vec{k},\vec{k}') = W(\vec{k}',\vec{k})$$

$$\left(\frac{\partial f}{\partial t}\right)_{scattering} = \int \left[f(\vec{k}') - f(\vec{k})\right] W(\vec{k},\vec{k}') \frac{d^3k'}{(2\pi)^3} \cdot V$$

$$= \int \left[\left(f(\vec{k}') - f^0(\vec{k}')\right) - \left(f(\vec{k}) - f^0(\vec{k})\right)\right] W(\vec{k},\vec{k}') \frac{d^3k'}{(2\pi)^3} \cdot V$$

$$= \int \left[g(\vec{k}') - g(\vec{k})\right] W(\vec{k},\vec{k}') \frac{d^3k'}{(2\pi)^3} \cdot V \qquad (52)$$

Steady state: $\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right) e\vec{v}(\vec{k})\cdot\vec{\mathcal{E}} = -\left(\frac{\partial f}{\partial t}\right)_{scattering} = \int\left[g(\vec{k})-g(\vec{k}')\right] W(\vec{k},\vec{k}')\frac{d^3k'}{(2\pi)^3}\cdot V$ (53)

But we introduced the relaxation time via:

$$\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right) e\vec{v}(\vec{k})\cdot\vec{\mathcal{E}} = -\left[-\frac{g(\vec{k})}{\tau}\right] \Rightarrow g(\vec{k}) = \left(-\frac{\partial f^0}{\partial \mathcal{E}}\right) e\tau\,\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}$$

(substitute into Eq. (53))

$$\left(-\frac{\partial f^0}{\partial \mathcal{E}}\right) e\vec{v}(\vec{k})\cdot\vec{\mathcal{E}} = -\left(\frac{\partial f^0}{\partial \mathcal{E}}\right) e\tau\;\vec{\mathcal{E}}\cdot\int\left(\vec{v}(\vec{k})-\vec{v}(\vec{k}')\right) W(\vec{k},\vec{k}')\frac{d^3k'}{(2\pi)^3}\cdot V$$

(τ still can be $\tau(\vec{k})$; $\vec{k}'$ over)

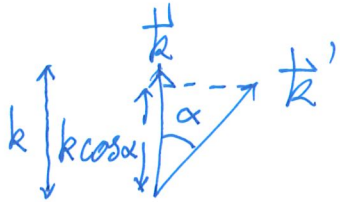
$$\Rightarrow \vec{v}(\vec{k})\cdot\vec{\mathcal{E}} = \tau\int\left(\vec{v}(\vec{k})-\vec{v}(\vec{k}')\right) W(\vec{k},\vec{k}')\frac{d^3k'}{(2\pi)^3}V\cdot\vec{\mathcal{E}}$$

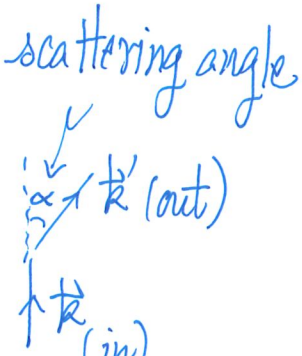
$$\Rightarrow \frac{1}{\tau} = \int W(\vec{k},\vec{k}')\left[1-\frac{\vec{v}(\vec{k}')\cdot\vec{\mathcal{E}}}{\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}}\right]\frac{d^3k'}{(2\pi)^3}\cdot V \qquad (54)$$

$\frac{1}{\tau(\vec{k})}$ formally; some angle; $|\vec{v}(\vec{k})| = |\vec{v}(\vec{k}')|$ (isotropic band)

The end result is (details omitted):

$$\frac{1}{\tau} = \int W(\vec{k},\vec{k}')\,(1-\cos\alpha)\,\frac{d^3k'}{(2\pi)^3}\cdot V \qquad (55)$$





Physics: small α, $\vec{k}'$ is in general still in the direction of $\vec{k}$

$\Rightarrow$ small angle elastic collisions are <u>not effective</u> in changing the direction of an electron

(not effective in giving rise to resistance)

$W(\vec{k},\vec{k}')$ has to be weighted by $(1-\cos\alpha)$ to account for the effectiveness of the $\vec{k}\to\vec{k}'$ process in randomizing the motion of an electron (against the effect of $\vec{F}_{ext}$)

Eq.(55) expresses this piece of physics, leaving $W(\vec{k},\vec{k}')$ for a separate QM calculation.

General aspect of Inelastic Collisions

- Can't do much that is general for metals and semiconductors ($W(\vec{k},\vec{k}') \neq W(\vec{k}',\vec{k})$)
- Non-degenerate semiconductors: See Eq.(51), $1-f(\vec{k}) \approx 1$, $1-f(\vec{k}') \approx 1$

$$\left(\frac{\partial f}{\partial t}\right)_{\text{inelastic}} = \int \left[f(\vec{k}')\,W(\vec{k}',\vec{k}) - f(\vec{k})\,W(\vec{k},\vec{k}')\right] \frac{d^3k'}{(2\pi)^3}\cdot V$$

$$= \int \left[\left(f^0(\vec{k}') + g(\vec{k}')\right)W(\vec{k}',\vec{k}) - \left(f^0(\vec{k}) + g(\vec{k})\right)W(\vec{k},\vec{k}')\right] \frac{d^3k'}{(2\pi)^3}\cdot V$$

$$= \int \left[g(\vec{k}')\,W(\vec{k}',\vec{k}) - g(\vec{k})\,W(\vec{k},\vec{k}')\right] \frac{d^3k'}{(2\pi)^3}\cdot V$$

$$= \int \left[g(\vec{k}')\frac{f^0(\vec{k})}{f^0(\vec{k}')} - g(\vec{k})\right] W(\vec{k},\vec{k}')\,\frac{d^3k'}{(2\pi)^3}\cdot V$$

$$= -\frac{g(\vec{k})}{\tau(\vec{k})} \quad \text{(in relaxation time approximation)}$$

Equilibrium terms give nothing

$f^0(\vec{k}')\,W(\vec{k}',\vec{k})$ → prob. $\vec{k}'$ is occupied

$= f^0(\vec{k})\,W(\vec{k},\vec{k}')$ ← prob. $\vec{k}$ is occupied

$$\frac{1}{\tau_{inelastic}} = \int \left[1 - \frac{g(\vec{k}')\, f^0(\vec{k})}{g(\vec{k})\, f^0(\vec{k}')}\right] W(\vec{k},\vec{k}') \frac{d^3k'}{(2\pi)^3} \cdot V \quad (55)$$

non-degenerate gas

another weighting factor

- $W(\vec{k},\vec{k}')$ (inelastic) is a separate calculation
- Boltzmann Equation is usually solved numerically for serious applications

What do we have so far?

- Putting details into $W(\vec{k},\vec{k}')$
- Need $W(\vec{k},\vec{k}')$ for various scattering processes (transport; optical properties)

QM enters → Fermi Golden Rule (works on electron-phonon, electron-photon processes)

→ Born Approximation

- For different processes i, $\frac{1}{\tau} = \sum_{\text{processes } i} \frac{1}{\tau_i}$

- Then, it is $\bar{\tau} = \frac{\langle \tau v^2 \rangle_0}{\langle v^2 \rangle_0} = \frac{\langle (\varepsilon - E_c)\tau(\varepsilon) \rangle_0}{\langle (\varepsilon - E_c) \rangle_0}$

  $\mu_e = \frac{e\bar{\tau}}{m_e^*}$

  that goes into the mobility μ_e and conductivity σ $(\sigma = ne\mu_e)$

- When both electrons and holes are present, they have different τ's

  $\Rightarrow$ different μ_e and μ_p

  $\sigma = ne\mu_n + pe\mu_p$

What's left is $W(\vec{k}, \vec{k}')$!

how to obtain $W(\vec{k}, \vec{k}')$ and related $\frac{1}{\tau}$ for various processes

(a) Fermi Golden Rule : Time-dependent perturbation theory

- Killing many birds at once

  transport, optical.

  (QM topics: time-dependent perturbation theory, scattering theory)

$$\hat{H} = \hat{H}_0 \quad \text{(before } \hat{H}'(t) \text{ enters)} \qquad \hat{H}_0 \psi_{\vec{k}} = E_{\vec{k}} \psi_{\vec{k}}$$

($\psi_{\vec{k}}$: knowns)

$$\hat{H} = \hat{H}_0 + \hat{H}'(\vec{r},t) = \hat{H}_0 + \hat{H}' \qquad (5b)$$

$\hat{H}'(\vec{r},t)$: time-dependent in general, e.g. light ($\sin\omega t / \cos\omega t$) interacting with charges

- how electron interacts with stuffs beyond periodicity (c.f. effective mass theory)
- e.g. electron sees vibrating ions/atoms
- e.g. electron gets closer to an impurity and then moves (scattered) away, here $H'(\vec{r})$

For EM waves (photons) or Lattice Vibrations (phonons) contexts.

(inelastic as electron will exchange energy by absorbing/creating photons/phonons)

Absorption

destroy a quantum

f —
i • electron AND n quanta of $(\hbar\omega)$ photons (needs $n \neq 0$) (initial)

→ • f, — i electron AND $(n-1)$ quanta of photons (final)

$$\boxed{E_f = E_i + \hbar\omega}$$

absorb a photon

Emission

Create a quantum

i —
f • electron AND n quanta of $(\hbar\omega)$ photons (initial)

→ i —, • f AND $(n+1)$ quanta of photons (final)

$$\boxed{E_f = E_i - \hbar\omega}$$

emit a photon

Stimulated Emission: $n \neq 0$ emission related to n (easier to handle)

Spontaneous Emission: $n = 0$ (harder to handle, but can be treated)

• "photon" → "phonon" (OK) "Destroy or create phonons"

Question: $\psi_{initial}$ is the state before $\hat{H}'$ enters

What is the rate of making a transition due to $\hat{H}'(t)$ to another state ψ_{final}?

[$\hat{H}'(\vec{r},t)$ has sinusoidal time]

$$W_{if} = \frac{2\pi}{\hbar}\left|\int \psi_f^* \hat{H}'(\vec{r})\,\psi_i\, d^3r\right|^2 \delta(E_f - E_i \pm \hbar\omega) \qquad (57)$$

W_{if}: †(from i to f)

"+" ⇒ $E_f = E_i - \hbar\omega$ emits

"−" ⇒ $E_f = E_i + \hbar\omega$ absorbs

$\int d^3r$: spatial integral

$\left|\int \psi_f^* \hat{H}'(\vec{r})\,\psi_i\, d^3r\right|^2$: energy^2 (unit)

$\delta(E_f - E_i \pm \hbar\omega)$: $\frac{1}{\text{energy}}$

Units? $W_{if} \sim \frac{\text{energy}}{\hbar} \sim \text{frequency} \sim \frac{1}{\text{time}}$ thus a rate

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† This echoes $W(k,k')$, which is $W_{kk'}$. The δ-function came from integration over time and serves to enforce energy conservation when quantum ($\pm\hbar\omega$) is destroyed and created.

Often written as

$$W_{if} = \frac{2\pi}{\hbar} |\langle f|\hat{H}'|i\rangle|^2 \delta(E_f - E_i \pm \hbar\omega) \qquad (57a)$$

doesn't matter $|\langle i|\hat{H}'|f\rangle|^2$ or $|\langle f|\hat{H}'|i\rangle|^2$

If we care only about transitions Out of state ψ_i (don't care about which state system ends up as there can be many states with the required E_f)

$$W_i = \frac{2\pi}{\hbar} \sum_{\text{final states}} |\langle f|\hat{H}'|i\rangle|^2 \delta(E_f - E_i \pm \hbar\omega) \qquad (58)$$

$\sum_{\text{final states}} \delta(E_f - E_i \pm \hbar\omega) \Rightarrow$ Counting states with particular energy E_f

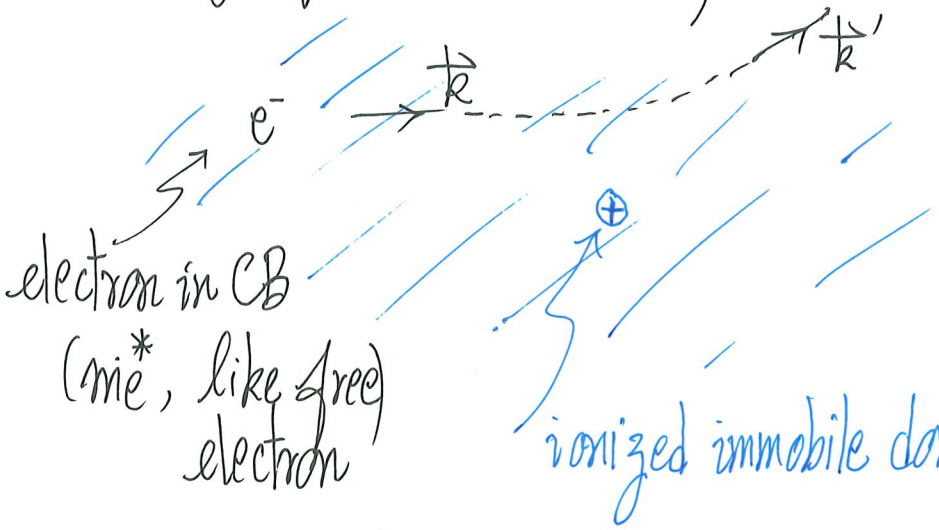
related to density of states $g(E_f)$

Eq. (58) is the key quantity in studying optical properties of solids

Logical sequence: $W_i \Rightarrow$ photons absorbed $\Rightarrow \alpha$ (absorption coefficient) $\Rightarrow \varepsilon_2$ ← imaginary part of dielectric function $\Rightarrow \varepsilon_1$ (Kramers-Kronig relation) $\Rightarrow$ Done

(b) By-product: Born Approximation

Scattering from some initially ψ_i to some final ψ_f by time-independent $\hat{H}'(\vec{r})$



"like Rutherford scattering" (but within a medium)

This is the Impurity Scattering problem of electrons in solids

dominating in semiconductors (together with el-phonon scattering)

$$W_{\vec{k}\vec{k}'} = W(\vec{k},\vec{k}') = \frac{2\pi}{\hbar} |\langle f|\hat{H}'|i\rangle|^2 \delta(E_{\vec{k}} - E_{\vec{k}'}) \qquad (59)$$

($\because \hat{H}'(\vec{r})$ only)

Born Approximation

for elastic scattering processes

If we only care about transitions out of state ψ_i,

$$W_i = \frac{2\pi}{\hbar} \sum_{\text{final states}} |\langle f|\hat{H}'|i\rangle|^2 \delta(E_f - E_i) = \frac{2\pi}{\hbar} \underbrace{|\langle f|\hat{H}'|i\rangle|^2}_{\text{often called } M_{if}} \underbrace{g(E_f)}_{\#/\text{energy (unit)}} \quad (E_f = E_i) \quad (66)$$

($\because g(\varepsilon)d\varepsilon = \#$)

Remarks:

- $W_i \propto g(E_f)$ ← More states to scatter into, higher W_i
- $\hat{H}'$ (e.g. $\sim -\frac{e^2}{r}$ or $-\frac{e^2}{r}e^{-\lambda r}$) doesn't alter spin of initial state

  $\Rightarrow$ $g(E_f)$ is for one particular spin

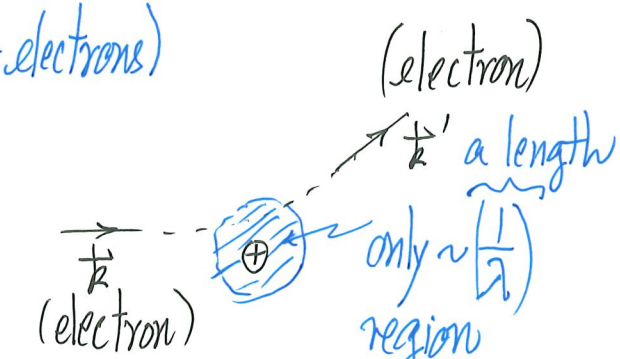
(c) Screened Coulomb Scattering as an example

- This is impurity scattering

$$U(\vec{r}) = \hat{H}'(\vec{r}) = \frac{Ze^2}{4\pi\varepsilon r} e^{-\lambda r} \qquad (61)$$

$e^{-\lambda r}$: screening (due to other electrons)

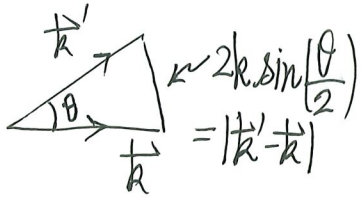
$\vec{0}$: impurity at $\vec{0}$



- We also this as an example to illustrate the sequence of calculations

$$M_{\vec{k}\vec{k}'} = \langle \vec{k}' | \hat{H}' | \vec{k} \rangle = \frac{Ze^2}{4\pi\varepsilon} \frac{1}{\sqrt{V}} \frac{1}{\sqrt{V}} \int e^{-i(\vec{k}'-\vec{k})\cdot\vec{r}} \frac{e^{-\lambda r}}{r} r^2 \sin\theta' \, d\theta' \, d\phi'$$

$(\vec{k}'-\vec{k})$ Fourier component of $U(r)$



$$= \frac{Ze^2}{\varepsilon} \frac{1}{V} \frac{1}{|\vec{k}'-\vec{k}|^2 + \lambda^2}$$

$$= \frac{Ze^2}{\varepsilon} \frac{1}{V} \frac{1}{4k^2 \sin^2\left(\frac{\theta}{2}\right) + \lambda^2}$$

($\lambda = 0 \Rightarrow$ unscreened Coulomb
$U_q \sim \frac{1}{q^2}$ is Fourier transform of $\sim \frac{1}{r}$)

c.f. Rutherford scattering ($\lambda = 0$)

$$W_{\vec{k}\vec{k}'} = W(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left(\frac{Ze^2}{V\varepsilon}\right)^2 \frac{1}{\left[4k^2\sin^2\left(\frac{\theta}{2}\right)+\lambda^2\right]^2} \cdot \delta(E_{\vec{k}} - E_{\vec{k}'}) \quad (62)$$

($|M_{\vec{k}\vec{k}'}|^2$)

Remarks

(i) $\lambda \to 0$ (unscreened) ← strong bias in small θ (forward) scattering

$$W(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left(\frac{Ze^2}{V\varepsilon}\right)^2 \frac{1}{16k^4\sin^4\left(\frac{\theta}{2}\right)} \cdot \delta(E_{\vec{k}} - E_{\vec{k}'})$$

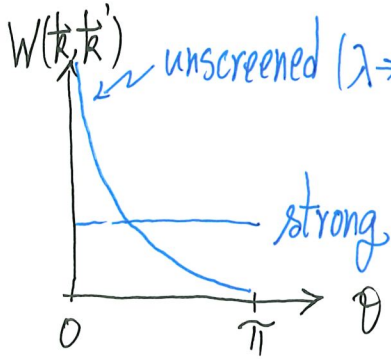
recall: used in interpreting α-particle scattering off gold film to establish existence of nuclei (Rutherford)

(ii) $\lambda \to \infty$ (strong screening, extremely short-range)

$$W(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left(\frac{Ze^2}{V\varepsilon}\right)^2 \frac{1}{\lambda^4} \cdot \delta(E_{\vec{k}} - E_{\vec{k}'})$$

(no angular dependence)

λ = 1/screening length [λ is NOT wavelength]



This is why we need to weight $W(\vec{k},\vec{k}')$ by $(1-\cos\theta)$ for scatterings into those $\vec{k}'$s (with bigger angles) effective for resistance (changing direction)

$$\frac{1}{\tau} = \underbrace{\int \frac{V}{(2\pi)^3}}_{\text{serve to sum over final states}} \underbrace{(1-\cos\theta)}_{\text{larger angle scatterings shorten } \tau} W(\vec{k},\vec{k}') \underbrace{d^3k'}_{\text{(see Eq. (55))}}$$

$$= \frac{2\pi}{\hbar}\left(\frac{Ze^2}{\varepsilon}\right)^2 \frac{1}{V^2}\frac{V}{(2\pi)^3}\int (1-\cos\theta)\,\frac{\delta(E_{\vec{k}}-E_{\vec{k}'})}{\left[4k^2\sin^2\left(\frac{\theta}{2}\right)+\lambda^2\right]^2}\, k'^2 \sin\theta\, dk'\, d\theta\, d\phi$$

$\vdots$ (many steps)

$$= \frac{\pi}{4\hbar}\left(\frac{Ze^2}{\varepsilon}\right)^2 g(E_{\vec{k}})\frac{1}{V^2k^4}\left[\ln\left(1+\left(\frac{2k}{\lambda}\right)^2\right) - \frac{1}{1+\left(\frac{\lambda}{2k}\right)^2}\right]$$

(it can be done!)

parabolic band $E_{\vec{k}} = \frac{\hbar^2k^2}{2m^*}$

$\Downarrow$

changing k'^2dk' integration to $dE_{k'}$ involving $g(E_k)$ (DOS)

where $g(E_{\vec{k}})$ = Density of states at electron energy $E_{\vec{k}}$ (for one kind of spin)

(not per unit volume)

$$= \frac{V}{4\pi^2} \cdot \boxtimes \left(\frac{2m^*}{\hbar^2}\right)^{3/2} \sqrt{E_k} \qquad = \frac{V}{\sqrt{2}} \frac{m^{*3/2}}{\pi^2 \hbar^3} \sqrt{E_k}$$

not so!

(∵ mechanism doesn't flip spin)

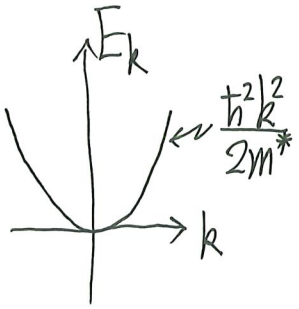
We emphasized earlier that $\tau(E)$. We can write τ in terms of $E_{\vec{k}}$.

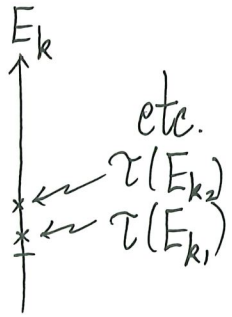
$$\frac{1}{\tau} = \left(\frac{Ze^2}{\varepsilon}\right)^2 \frac{1}{V} \cdot \frac{1}{16} \frac{1}{\sqrt{2}\pi} \frac{1}{\hbar^4 k^4} \cdot m^{*3/2} \sqrt{E_k} \cdot \left[\ln\left(1 + \frac{8m^* E_{\vec{k}}}{\hbar^2 \lambda^2}\right) - \frac{1}{1 + \frac{\hbar^2 \lambda^2}{8m^* E_{\vec{k}}}} \right]$$

$$= \left(\frac{Ze^2}{\varepsilon}\right)^2 \frac{1}{V} \frac{1}{16} \frac{1}{\sqrt{2}\pi} \frac{1}{m^{*1/2} E_{\vec{k}}^{3/2}} \cdot \left[\ln\left(1 + \frac{8m^* E_{\vec{k}}}{\hbar^2 \lambda}\right) - \frac{1}{1 + \frac{\hbar^2 \lambda^2}{8m^* E_{\vec{k}}}} \right] \qquad (63)$$

Now, we see that we really have $\tau(E_{\vec{k}})$ due to screened ionized impurity scattering!

(Scattering potential parameterized by λ)





Not done yet! Why? The story goes...

- Electrons are populated in equilibrium by f^0
- Equilibrium f^0 is modified by $\vec{\mathcal{E}}$ (driving force: electric field) to $f^0 + \delta f$

drift velocity gives $\vec{v}$ and $\vec{j}$

μ = mobility $= \dfrac{e\bar{\tau}}{m^*}$ with $\bar{\tau} = \dfrac{\langle v^2 \tau \rangle_0}{\langle v^2 \rangle_0}$ where $\langle \cdots \rangle_0 = \dfrac{\int_0^\infty (\cdots) v^2 e^{\frac{-m^* v^2}{2kT}} dv}{\int_0^\infty v^2 e^{\frac{-m^* v^2}{2kT}} dv}$

(Boltzmann Transport Theory)

"kT" will enter

- Getting $\bar{\tau}$ is a long calculation! (but it can be done!)

$$\bar{\tau} = \frac{\langle v^2 \tau \rangle_0}{\langle v^2 \rangle_0} = \frac{\langle E \tau(E) \rangle_0}{\langle E \rangle_0}$$

using $f^0(E) \sim e^{-E/kT}$

$\Rightarrow$ end result $\bar{\tau}$ has kT in it (and E_k integrated over)

The end result is:

$$\frac{1}{\tau} = \frac{1}{128\sqrt{2\pi}} \frac{1}{V} \left(\frac{Ze^2}{\varepsilon}\right)^2 \frac{1}{m^{*1/2}(kT)^{3/2}} \cdot \left[\ln\left(1+\frac{24m^*kT}{\hbar^2\lambda^2}\right) - \frac{1}{1+\frac{\hbar^2\lambda^2}{24m^*kT}}\right] \qquad (64)$$

Done!? Done for <u>one single scatterer</u>

To complete the discussion, consider N_d (or N_{imp}) impurites <u>per unit Volume</u>

∴ there are a total of $N_{imp} \cdot V$ ionized impurities (scatterers) in system

∴

$$\frac{1}{\tau} = \underbrace{\frac{N_{imp}}{128\sqrt{2\pi}} \left(\frac{Ze^2}{\varepsilon}\right)^2 \frac{1}{m^{*1/2}(kT)^{3/2}}}_{\text{this has unit of } \frac{1}{\text{time}}} \cdot \left[\ln\left(1+\frac{24m^*kT}{\hbar^2\lambda^2}\right) - \frac{1}{1+\frac{\hbar^2\lambda^2}{24m^*kT}}\right] \qquad (65)$$

(scatterers work independently)

Really done! Putting together fundamental QM, transport theory, statistical physics, scattering mechanism, AND patience, it is possible to get at measureable quantities.

- An interesting observation...

  from $\tau(E_k)$ to $\overline{\tau}$

  ↘ take $\tau(E_k)$ and go to $\underbrace{\tau(kT)}_{\approx \overline{\tau}}$ (∵ kT is representative of energy in a non-degenerate gas)

  ↓ ↙

  see Eq. (63) and Eq. (64)

  This saves many steps!

- More impurities (N_{imp}) $\overline{\tau} \sim \frac{1}{N_{imp}} \Rightarrow \overline{\tau}$ drops and μ drops

  (μ: mobility)

  $\sigma = ne\mu$ may increase as n is increased by having more donors

Finally, $\mu = \frac{e\bar{\tau}}{m^*}$ ← from Eq. (65)

$\bar{\tau} \sim (kT)^{3/2}$ in prefactor

∴ If ionized impurities are the dominant scattering process

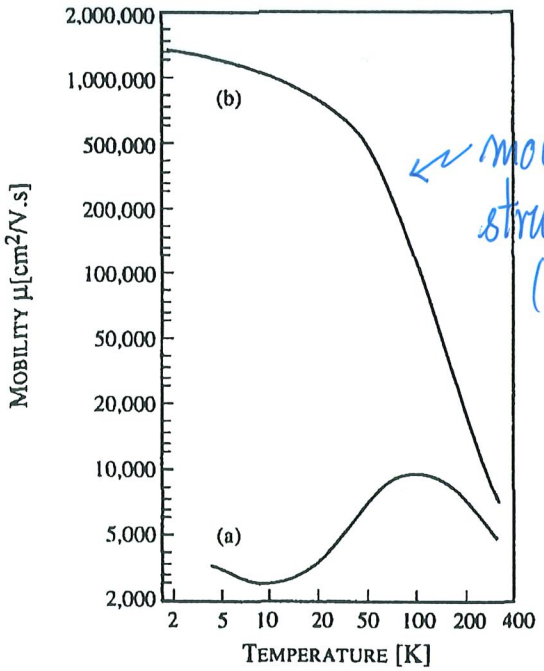
(temperature not too high so that phonon mechanism is not important

but yet temperature (1 meV scale) is sufficient to ionize donors/acceptors),

expected to see $\mu \sim T^{+3/2}$

but actual situation is more complicated

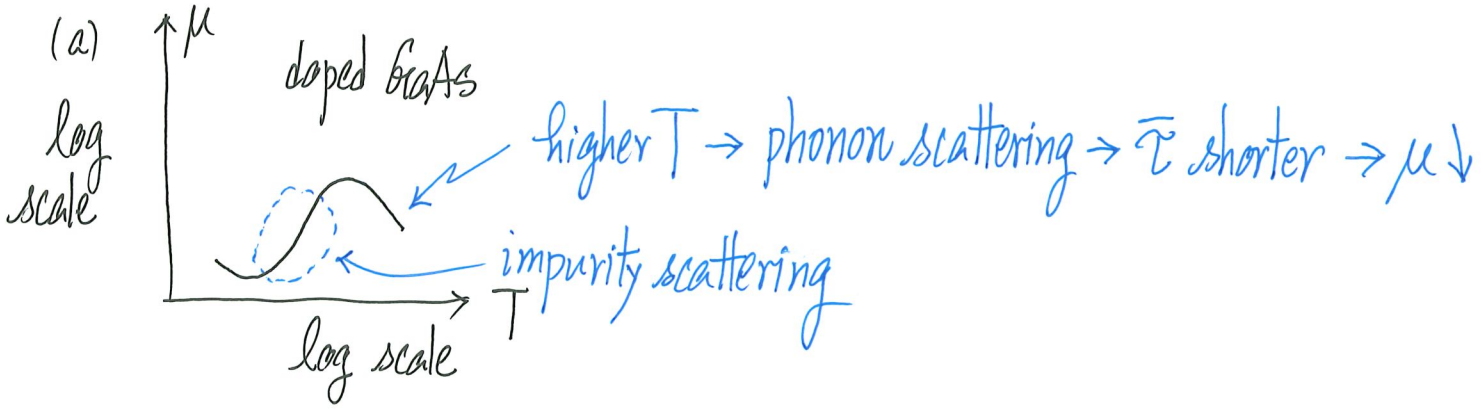
[other mechanisms, other "kT" terms in result]



← modulation-doped structure (avoid effective head-on collisions)

A typical plot of electron mobility as a function of temperature in a uniformly doped GaAs with $N_D = 10^{17}$ cm^{-3}. The mobility drops at low temperature due to ionized impurity scattering, becoming very strong. In contrast, the curve *b* shows a typical plot of mobility in a modulation-doped structure where ionized impurity is essentially eliminated.

Taken from J. Singh, "Physics of Semiconductors and their Heterostructures"



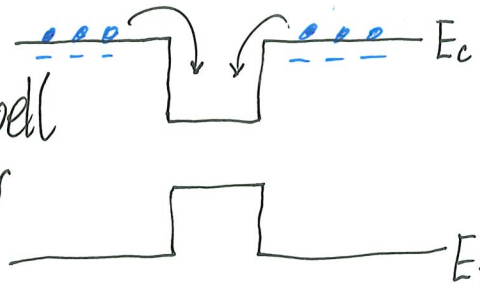
High-Mobility Structures

- μ is suppressed by impurity scatterings that change the direction
  (small-angle ones don't matter)
- For higher μ, avoid such collisions
  how? separate electrons (carriers) from ionized impurities in space

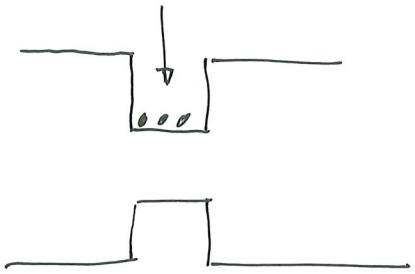
Heterostructures

dope here ↑ ↖ dope here

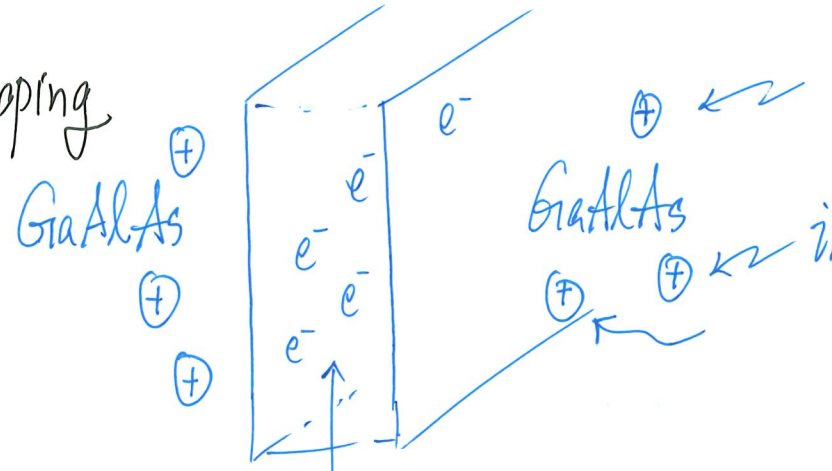
electrons go into well as energy is lower



electrons live in sandwiched layer



Modulation doping



immobile ionized donors are in GaAlAs regions

electrons move "freely" inside GaAs

electrons will not collide with ionized donors head-on and change direction

$\Rightarrow$ high mobility

Even 2D Electron gas (quantum Hall effect) is constructed using this idea.

(d) Other Processes

(i) Alloy Scattering

GaAs periodic $Ga_{1-x}Al_xAs$ $x = 0.2$

20% of cation sites have Al
80% of cation sites have Ga

Construct a (unreal) periodic system will virtual cations (averaged Ga and Al)
(Virtual crystal approximation)[+] Bloch states, band structure, ...

Then there are deviations at every cation site ⇒ alloy scattering
(this is elastic)

Treated in similar way as impurity scattering

$$\frac{1}{\tau} \sim x(1-x)(kT)^{1/2}$$ giving $\mu_{alloy} \sim T^{-1/2}$

[+] Alloys have two interesting treatments: VCA and CPA (coherent potential approximation)

(ii) Lattice Vibrations (Phonons)

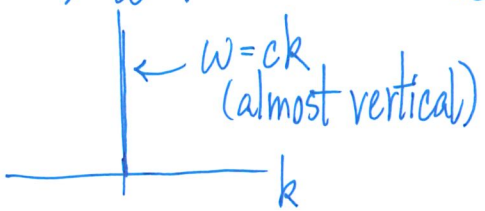
- Similarity between electron-photon and electron-phonon scatterings
  - photon: oscillators
  - phonon: oscillators
  - absorb and create quantum
  - stimulated and spontaneous emission (creation of photon)

But

photons

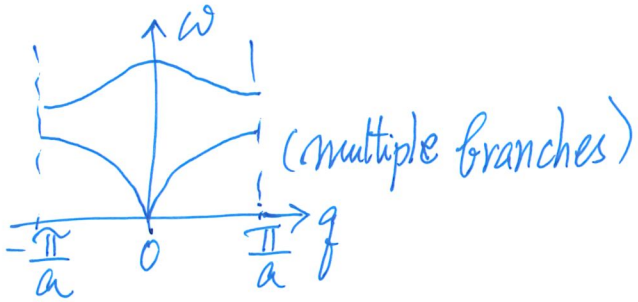
$k = \frac{\omega}{c}$

k: tiny compared with $\frac{\pi}{a}$ (B.Z. size)



n_ω is related to intensity of light at frequency ω

phonons



$\left(n_\omega + \frac{1}{2}\right)\hbar\omega$ for mode with ω

n_ω: $n_\omega(T) = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$ depends on T

Normal mode involves motion of every atom

$$u_{i^{th}\,atom,\vec{q}}(t) = u_{0i}\, e^{i(\vec{q}\cdot\vec{r}_i - \omega t)}$$

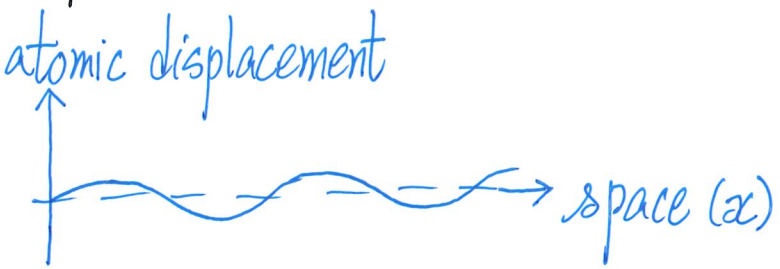
- $u_{i^{th}\,atom,\vec{q}}(t)$: displacement at time t
- $\omega(q)$: mode
- u_{0i}: amplitude
- $\vec{r}_i$: where atom i is

Broadly speaking: Acoustic branches - Atoms in unit cell move with same sign

Optical branches - Atoms in unit cell move with opposite signs

These motions produce disturbances (deviations) that can scatter electrons

Pictures:



These displacements are like shearing (acoustic modes) and squeezing the crystal locally ⇒ creating local potential disturbances

Acoustic modes

electron scattered by "deformation" (locally deformed)

$$U_{acoustic} \sim \underbrace{D}_{\text{deformation potential (eV)}} \frac{\partial u}{\partial x} \qquad (66)$$

(time-dependent)

Optical modes

atoms in unit cell move in opposite directions

$\Rightarrow$ create potential disturbance $\sim u$

$$U_{optical} \sim D_0 u \qquad (67)$$

D_0: optical deformation potential (eV/cm)

Optical Modes with Cations and Anions

- Considered earlier for their optical effect (polariton)
- effective $+e^*$ ion and $-e^*$ ion $\Rightarrow$ polarization fields

$$U_{\text{polarization(optical)}} \sim e^* u \qquad (68)$$

All effects $\sim u \sim (\hat{a}^+ + \hat{a}) \Rightarrow$ processes can create/destroy phonon

energy consideration: $E_f = E_i \pm \hbar\omega$

momentum consideration: $\hbar\vec{k}_f = \hbar\vec{k}_i \pm \hbar\vec{q}$ (could include $\pm\hbar\vec{G}$)

Acoustic phonon scattering

$q \to 0$, $\omega \to 0$ (phonon energy is small $\Rightarrow$ electron's energy doesn't change by much)

$W^{acoustic}(E_k)$ = Scattering rate for an electron with energy E_k to other states

$$= \frac{2\pi D^2}{\hbar} \frac{kT}{\rho v_s^2} \cdot g(E_k) \qquad (69)$$

- $g(E_k)$: DOS
- v_s: speed of sound
- ρ: mass density of semiconductor

Optical phonon scattering

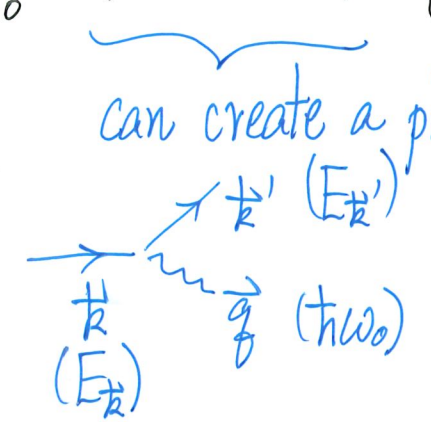
$$W^{absorption}(E_k) = \frac{\pi D_0^2}{\rho \omega_0} n(\omega_0)\, g(E_k + \hbar\omega_0) \qquad (70)$$

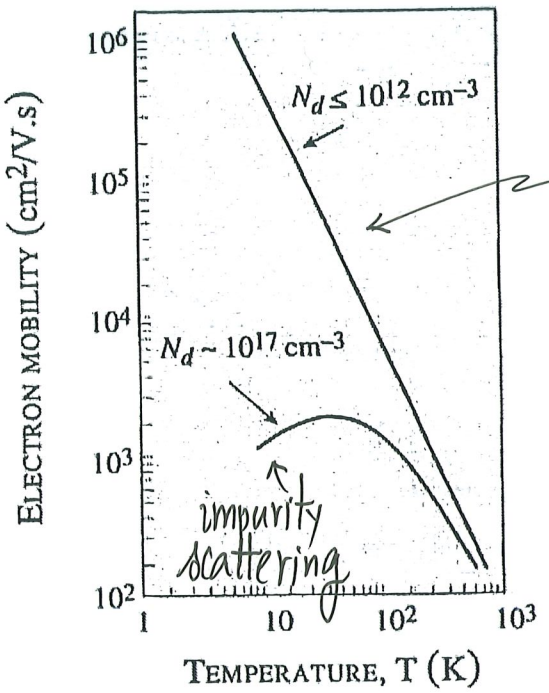
- $g(E_k + \hbar\omega_0)$: DOS at $E_f = E_k + \hbar\omega_0$
- $n(\omega_0)$: # phonons (temperature dependent)
- $E_k + \hbar\omega_0$: absorbs a phonon
- ω_0 = optical mode frequency

$$W^{\text{create phonon}}(E_{\vec{k}}) = \frac{\pi D_0^2}{\rho \omega_0} \cdot \underbrace{(n(\omega_0) + 1)}_{\text{can create a phonon even there is no phonon around}} \cdot g(E_{\vec{k}} - \hbar\omega_0) \qquad (71)$$

$(n(\omega_0) = 0)$

"spontaneous emission"





Mobility of electrons in silicon as a function of doping and temperature.

μ increases as T decreases
because phonon scattering is less important as T decreases
and no impurity scattering for low N_d

	Bandgap (eV)	Mobility at 300 K (cm^2/V-s)	
Semiconductor	300 K	Electrons	Holes
C	5.47	800	1200
Ge	0.66	3900	1900
Si	1.12	1500	450
α-SiC	2.996	400	50
GaSb	0.72	5000	850
GaAs	1.42	8500	400
GaP	2.26	110	75
InAs	0.36	33000	460
InP	1.35	4600	150
CdTe	1.56	1050	100

Bandgap, electron, and hole mobilities of some semiconductors. Notice that narrow bandgap materials have superior mobility, since the effective mass is smaller.

From J Singh, "Physics of Semiconductors and their Heterostructures"

Final Remarks

- High-Field Transport
  - Easy to have High-field ($\vec{\mathcal{E}}$-field) as semiconductor structures shrink in size
  - Hot electron, non-linear behavior $\mu(\mathcal{E})$

Refs

- Elliot and Gibson, "An introduction to Solid State Physics and its Applications"
  (simple coverage on Boltzmann Theory with discussions on semiconductors)
- McKelvey, "Solid State Physics for Engineering and Materials Science" Ch. 7, 9
- J. Singh, "Physics of Semiconductors and their Heterostructures", chapters on scattering processes
- Smith, "Semiconductors"