ECE 5390 / MSE 5472, Fall Semester 2017

Quantum Transport in Electron Devices and Novel Materials

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Assignment 3, Solutions

Problem 3.1: Designer digital and analog ballistic FETs

Problem 3.1) Designer digital and analog Ballistic FETs

In class we discussed that for a Ballistic FET with a 2D electron gas channel, a parabolic bandstructure $E(k_x, k_y) = \frac{\hbar^2}{2m^\star}(k_x^2 + k_y^2)$ leads to a current $\frac{I_d}{W} \propto (V_{gs} - V_T)^{\frac{3}{2}}$, leading to a gain or transconductance $g_m = \frac{\partial I_d}{\partial V_{gs}} \propto (V_{gs} - V_T)^{\frac{1}{2}}$.

(a) Using the on-state current as the primary metric, discuss the effects of the band-edge effective mass $m^\star$ and k-valley degeneracy g_v on the FET on-current. Using your program for Problem 2.6 in Assignment 2, show that the dependence can be *non-monotonic*, meaning a lighter effective mass does guarantee the highest on-current, and a higher valley degeneracy does not always mean a higher on-current. What is the reason?

(b) Show why if the gate of the FET is driven by a monochromatic input signal $V_{gs} = V_{gs}^{dc} + v_\omega e^{i\omega t}$, the output ac current has many frequencies, not just the frequency of the input signal.

(c) Assume $v_\omega << V_{gs}^{dc}$. Can you design a bandstructure that will remove these higher harmonics? This will make the transistor more linear. If you have a good strategy, you can make an impact on communication electronics, where transistors with high *linearity* are in demand.

Solution:

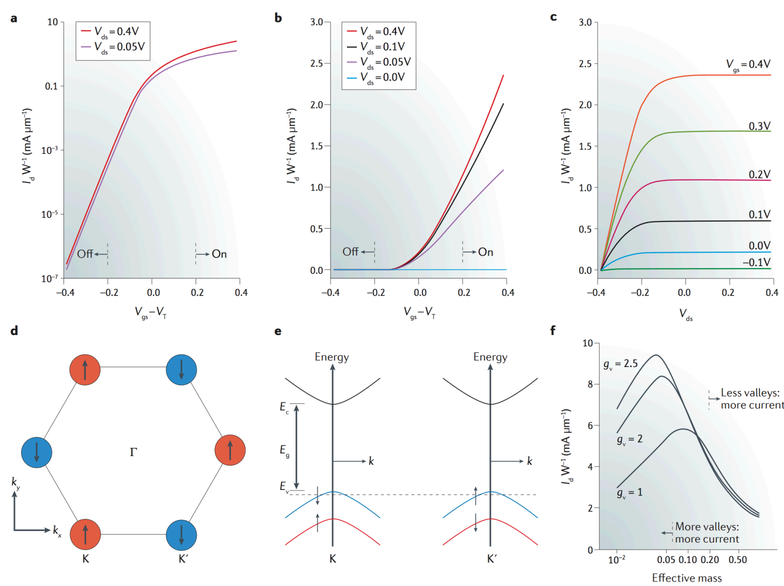


Figure 3 | **Calculated FET characteristics and spin–valley locking in the valence band of 2D TMDs.** The output characteristics of a transition metal dichalcogenide (TMD) ballistic field-effect transistor (FET) with $m_c^* = 0.5m_0$, $\varepsilon_b = 20\varepsilon_0$ and $t_b = 3$ nm are calculated (panels **a–c**). **a** | Transfer characteristics with the drain current, I_d, in logarithmic form for two different drain voltages (V_{ds}). **b** | Transfer characteristics in linear from at different drain voltages. **c** | Calculated output characteristics of a prototype ballistic 2D semiconductor channel FET at different gate voltages. Note that these calculations do not consider contact resistances. **d** | The electronic structure of a unit cell — referred to as the first Brillouin zone — of monolayer MoS_2. The high symmetry points (K, K′ and Γ) of the unit cell in the momentum space are indicated. The K and K′ points are two inequivalent momentum valleys: the energy maxima and minima. The arrows indicate spins of the valence electrons occupying that valence state. $k_{x,y}$ are the wavevectors that represent the direction of electron wavefunction propagation. **e** | The valence band splits at these valleys as a consequence of strong spin–orbit coupling. Time reversal symmetry requires spins to be opposite at different valleys. **f** | Drain current as a function of effective mass for three different values of valley degeneracy (g_v). The drain currents were obtained for V_{gs} and V_{ds} = 0.4 V. The cross-over of current scaling with valleys and effective mass depends on the gate capacitance.

(a) Here is a calculation that I had done recently for a review paper. Fig (f) shows how the maximum on current depends on the band effective mass, and the valley degeneracy. For example for a single valley, an effective mass of ~0.1m0 gives the highest on-state ballistic current drive. Note that I have assumed that the bands are isotropic for the calculation, that is another parameter one could vary further to squeeze out more performance in ballistic FETs. Also, note that the calculation neglects the effect of contact resistances (this effect can be strong, and current densities of Id~10 mA/um are not possible at small voltages because a quantum-limited contact resistance of Rc~50 Ohm-um will still 2*Id*Rc ~ 1.0 Volt , with Id*Rc dropping at each contact. Though this contact effect will stretch out the Id-Vgs and Id-Vds curves, and limit the current drive, it will not change the fundamental observation that there is an optimal effective mass for any given valley degeneracy.

(b)

$$\frac{I_d}{W} \propto (V_{gs} - V_T)^{3/2} \; ; \quad \text{Say} \quad V_{gs} = (V_{gs}^{dc} + V_w e^{i\omega t})$$

$$\Rightarrow \frac{I_d}{W} \propto (V_{gs}^{dc} - V_T + V_w e^{i\omega t})^{3/2} . \quad \text{Taylor expansion about } V_w = 0,$$

$$\Rightarrow \frac{I_d}{W} \propto (V_{gs}^{dc} - V_T)^{3/2} + \frac{3}{2}\sqrt{V_{gs}^{dc} - V_T}\, V_w e^{i\omega t} + \underbrace{\frac{3/8}{\sqrt{V_{gs}^{dc} - V_T}}\, V_w^2 e^{i2\omega t} + \ldots}_{\text{harmonics}}$$

(c)

Say $E(k) = \frac{\hbar^2}{2m^*} k^n$.

$$J_{2d} = \frac{q g_s g_v}{(2\pi)^2} \iint d^2k \, \bar{v}_g(\bar{k}) f(\bar{k}) \; ; \quad \bar{v}_g(\bar{k}) = \frac{1}{\hbar} \nabla_k E(k) = \frac{\hbar}{2m^*} n k^{n-1} \underbrace{\hat{k}}_{\text{unit vector}}$$

Go through the standard derivation to get

$$J_{2d}^n = \frac{q g_s g_v}{(2\pi)^2} \left(\frac{2k_BT}{\hbar}\right) \left(\frac{\hbar^2}{2m^* k_BT}\right)^{-1/n} \; ; \quad v_d = \frac{q V_{DS}}{k_BT} \; ;$$

$$J_{2d} = J_{2d}^n \left[\mathcal{F}_{1/n}(\eta_s) - \mathcal{F}_{1/n}(\eta_s - v_d) \right] \cdot \Gamma\left(\frac{1}{n} + 1\right)$$

For $\eta_s >> 1$, $\mathcal{F}_j(\eta) \simeq \frac{\eta^{j+1}}{\Gamma(j+2)}$

$\eta_s \to 2\eta_g$, where $\eta_g = \frac{C_b}{C_b + C_q}\left(\frac{V_{gs} - V_T}{V_{th}}\right)$

$$\therefore J_{2d} \sim J_{2d}^n \mathcal{F}_{1/n}(2\eta_g) \Gamma\left(\frac{1}{n} + 1\right)$$

$$= J_{2d}^n 2^{\frac{1}{n}+1} \frac{\Gamma\left(\frac{1}{n}+1\right)}{\Gamma\left(\frac{1}{n}+2\right)} \left(\frac{C_b}{C_b + C_q}\right)^{\frac{1}{n}+1} \left(\frac{V_{gs} - V_T}{V_{th}}\right)^{\frac{1}{n}+1}$$

$$\Rightarrow \boxed{J_{2d} \propto (V_{gs} - V_T)^{1+1/n}}$$

If we want a purely linear behaviour, $n \to \infty$ which is not easy to achieve in practice.

* Say $n = 1$, then

$$J_d \propto (V_{gs} - V_T)^2$$
$$\propto (V_{gs}^{dc} - V_T + v_w e^{i\omega t})^2$$
$$= (V_{gs}^{dc} - V_T)^2 + 2 v_w (V_{gs}^{dc} - V_T) e^{i\omega t} + \underbrace{v_w^2 e^{i2\omega t}}_{\text{higher order}}$$

However if $V_{gs}^{dc} >> v_w$, then the $v_w^2(\ )$ is small $\Rightarrow$ the output is approximately linear.

Problem 3.2: The Boltzmann Transport Equation

Problem 3.2) The Boltzmann Transport Equation

In class, we discussed the Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = \hat{C} f \tag{1}$$

where the symbols have the usual meanings. The collision term on the right is

$$\hat{C} f = \sum_{k'} [S(k' \to k) f_{k'}(1 - f_k) - S(k \to k') f_k (1 - f_{k'})], \tag{2}$$

where $S(k \to k') = \frac{2\pi}{\hbar} |\langle k'|W(r)|k\rangle|^2 \delta(E_{k'} - E_k \pm \hbar\omega)$ are the scattering rates given by Fermi's golden rule. In this problem, we discuss a few details of this recipe of solving diffusive transport problems. For *any* scattering potential, we found that $\frac{S(k \to k')}{S(k' \to k)} = \exp(\frac{E_k - E_{k'}}{kT})$, which led us to distinguish between elastic and inelastic scattering events.

a) Under what conditions can we make the relaxation time approximation (RTA), where $\hat{C} f \approx -(f - f_0)/\tau$? Discuss for both elastic and inelastic scattering events.

b) Outline how from the RTA of the distribution function f, one may obtain charge transport properties such as the electrical conductivity, and thermoelectric properties.

c) For a force $\mathbf{F} = q\mathbf{F_e}$ due to an electric field *alone*, the RTA solution of the BTE took the form

$$f \approx f_0 + \tau(-\frac{\partial f_0}{\partial E}) \mathbf{v} \cdot \mathbf{F}. \tag{3}$$

However, in the presence of a crossed electric and magnetic field, the net force is the Lorentz force, $\mathbf{F} = q(\mathbf{F_e} + \mathbf{v} \cdot \mathbf{B})$. Work out a solution for f in the RTA for this situation. You may refer to Wolfe/Holonyak/Stillman's book on the Physics of Semiconductors for this part. Realize that this is the situation encountered in a Hall-effect measurement.

d) Outline how magnetoresistance properties may be obtained from the BTE from your discussion above.

Solution:

(a) The key to apply RTA is that τ_k does not depend on f.

assume f can be splitted into a symmetric and an antisymmetric part.

$$f = \underbrace{f_S}_{\text{symmetric}} + \underbrace{f_A}_{\text{anti-symmetric}}$$

$$-\frac{f-f_0}{\tau} = \sum_{\vec{k}'} \left[S(k' \to k) f'(1-f) - S(k \to \vec{k}') f (1-f') \right]$$

for non-degenerate case.
$$\begin{cases} 1-f \sim 1 \\ S(k \to k')/S(k' \to k) \sim \exp\left(\frac{E_k - E_{k'}}{kT}\right) \end{cases}$$

when the distribution is not far from equilibrium

$$f_S' \sim f_S \sim f_0 .$$

$$\Rightarrow \quad -\frac{f_A}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[\exp\left(\frac{E_{k'} - E_k}{kT}\right) f_A' - f_A \right]$$

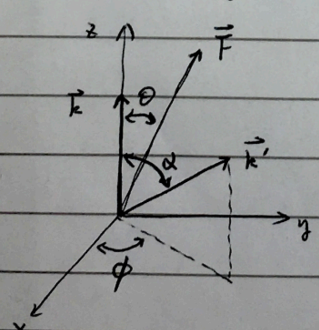
$$\Rightarrow \quad \frac{1}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[1 - \exp\left(\frac{E_{k'} - E_k}{kT}\right) \frac{f_A'}{f_A} \right]$$

for spherical bands under low fields. f_A has a general form.

(Ref Mark Lundstrom's book) $\quad f_A = g(k) \cos\theta .$

$$\Rightarrow \quad \frac{1}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[1 - \exp\left(\frac{E_{k'} - E_k}{kT}\right) \frac{g(k')}{g(k)} \frac{\cos'\theta}{\cos\theta} \right]$$

$\boxed{\text{Elastic Scattering}}$.



$$\frac{1}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[1 - \frac{\cos'\theta}{\cos\theta} \right]$$

$$\frac{\cos'\theta}{\cos\theta} = \tan\theta \sin\alpha \sin\phi + \cos\alpha .$$

Integral of $\sin\phi$ gives zero.

$$\Rightarrow \quad \frac{1}{\tau_k} = \sum_{\vec{k}} S(k \to k') \left[1 - \cos\alpha \right]$$

α: angle between $\vec{k}$ and $\vec{k}'$

$\Rightarrow \frac{1}{\tau_k}$: not depend on f.

$\boxed{\text{Inelastic Scattering}}$
$$\frac{1}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[1 - \exp\left(\frac{E_{k'} - E_k}{kT}\right) \frac{g(k')}{g(k)} \frac{\cos'\theta}{\cos\theta} \right]$$

$$\because g(k) \propto \left(\frac{\partial f}{\partial E}\right) k \quad \rightarrow \quad \frac{g(k')}{g(k)} = \exp\left(\frac{E_k - E_{k'}}{kT}\right) \frac{k'}{k}$$

$$\Rightarrow \quad \frac{1}{\tau_k} = \sum_{\vec{k}'} S(k \to k') \left[1 - \frac{k'}{k} \cos\alpha \right]$$

go back to $\frac{1}{\tau_k} = \sum_{k'} S(k \to k') \left[1 - \exp\left(\frac{E_{k'} - E_k}{kT}\right) \frac{f_{A'}}{f_A}\right]$

$\because$ f_A is not a function of k'

$f_{A'}$ is anti-symmetry.

for ~~spherical~~ band $E_{k'}$ is even in k'

$\therefore$ as long as $S(k \to k')$ is even in k'.

the integral of the ~~to~~ second term will vanish.

$\Rightarrow$. Isotropic scattering (no ~~matter~~ elastic or inelastic)

$\Rightarrow$. $$\frac{1}{\tau_k} = \sum_{k'} S(k \to k')$$

(b). Once we know f and τ:

electrical conductivity $\sigma = \frac{q^2 n \langle \tau_m \rangle}{m^*}$

(3D semiconductor) $$\langle \tau_m \rangle = \frac{2}{3} \frac{\int_0^\infty \tau_k (-\partial f / \partial x) x^{3/2} dx}{\int_0^\infty f_0 x^{1/2} dx}$$

Hall constant: $R_H = -\frac{1}{qn} \frac{\langle \tau^2 \rangle}{\langle \tau \rangle^2}$

Thermal conductivity due to electron:

$$\kappa = \frac{n}{m^* T} \left[\langle \tau e^2 \rangle - \frac{\langle \tau e \rangle^2}{\langle \tau \rangle}\right]$$

Thermoelectric Effects.

Thomson coefficient: $\mathcal{T} = T \frac{d}{dT}\left[\frac{\langle \tau e \rangle}{qT\langle \tau \rangle}\right]$

e = heat content per electron. $e = \mathcal{E} - E_F$

thermoelectric power: $\mathcal{P}$: $\mathcal{T} = -T \frac{d}{dT} \mathcal{P}$

$$\mathcal{P} = -\frac{\langle \tau e \rangle}{qT\langle \tau \rangle}$$

Peltier coefficient: $\Pi = -\frac{\langle \tau e \rangle}{q\langle \tau \rangle}$

(c). Ref. Charles Wolfe's book.

with crossed electric and magnetic field.

$$\frac{f - f_0}{\tau} = \frac{q}{\hbar}(\vec{E} + \vec{v} \times \vec{B}) \cdot \nabla_k f - \vec{v} \cdot \nabla_r f$$

assume the solution has the form of

$$f = f_0 + \tau \frac{\partial f_0}{\partial \mathcal{E}} \vec{v} \cdot \vec{G}$$

$\vec{G}$: a general force to solve.

$$\frac{f-f_0}{\tau} = \frac{\partial f_0}{\partial E}\vec{v}\cdot\vec{G} = \frac{q}{\hbar}(\vec{E}+\vec{v}\times\vec{B})\nabla_k f - \vec{v}\cdot\nabla_r f.$$

$$(\vec{E}+\vec{v}\times\vec{B})\cdot\nabla_k f = \hbar\frac{\partial f_0}{\partial \varepsilon}\vec{v}\cdot\vec{E} + \tau\frac{\partial f_0}{\partial \varepsilon}(\vec{v}\times\vec{B})\cdot\nabla_k(\vec{v}\cdot\vec{G})$$

$$\vec{v}\cdot\nabla_r f = kT\frac{\partial f_0}{\partial \varepsilon}\,\vec{v}\cdot\nabla_r\left(\frac{E-E_F}{kT}\right)$$

$$\Rightarrow \frac{\partial f_0}{\partial \varepsilon}\vec{v}\cdot\vec{G} = q\frac{\partial f_0}{\partial \varepsilon}\vec{v}\cdot\vec{E} - kT\frac{\partial f_0}{\partial \varepsilon}\vec{v}\cdot\nabla_r\left(\frac{\varepsilon-E_F}{kT}\right) + \tau\frac{q}{\hbar^2}\frac{\partial f_0}{\partial \varepsilon}\vec{v}\cdot[\vec{B}\times(\vec{G}\cdot\nabla_k)\nabla_k\varepsilon]$$

$\Rightarrow$

$$\vec{G} = \underbrace{q\vec{E} - kT\nabla_r\left(\frac{\varepsilon-E_F}{kT}\right)}_{q\vec{\mathcal{F}}.} + \tau\frac{q}{\hbar^2}[\vec{B}\times(\vec{G}\cdot\nabla_k)\nabla_k\varepsilon]$$

$$\Rightarrow \vec{G} = q\vec{\mathcal{F}} + \frac{q\tau}{\hbar^2}[\vec{B}\times(\vec{G}\cdot\nabla_k)\nabla_k\varepsilon]$$

$$\Rightarrow \vec{G} = q\left[\frac{\vec{\mathcal{F}} - q\tau\,\vec{M}\cdot(\vec{\mathcal{F}}\times\vec{B}) + (q\tau)^2(\det\vec{M})(\vec{\mathcal{F}}\cdot\vec{B})(\vec{M}'\cdot\vec{B})}{1+(q\tau)^2(\det\vec{M})(\vec{M}^{-1}\cdot\vec{B})\cdot\vec{B}}\right]$$

M: effective mass tensor.

for spherical band.

$$f = f_0 + \frac{\partial f_0}{\partial \varepsilon}q\tau\vec{v}\cdot\left[\frac{\vec{\mathcal{F}} - (q\tau/m^*)(\vec{\mathcal{F}}\times\vec{B}) + (q\tau/m)^2(\vec{\mathcal{F}}\cdot\vec{B})\vec{B}}{1+(q\tau/m^*)^2\vec{B}\cdot\vec{B}}\right]$$

$\vec{\mathcal{F}}$ term : ohmic contribution $\rightarrow$ electrical and thermal conductivity and thermoelectric effects.

$\vec{\mathcal{F}}\times\vec{B}$: Hall contribution.

$\vec{B}^2$ term : magnetoresistive effects.

Problem 3.3: Applications of Fermi's Golden Rule: Scattering rates due to Point Defects, and Alloy Disorder Scattering

Problem 3.3) Application of Fermi's Golden Rule: Scattering rates due to Point Defects, and Alloy Disorder Scattering

Assume that in a 3D semiconductor crystal of GaN (electron effective mass = $m^{\star} \sim 0.2m_0$), point defects of volume density $n_{imp} = N_{imp}/V$ are present. Also, assume that the perturbation V_0 to the crystal potential due to each point defect is confined to a radius R_0 around its location, i.e.,

$$W(\mathbf{r}) = V_0 \theta(R_0 - |\mathbf{r}|), \tag{4}$$

where $\theta(...)$ is the unit-step function. This is an example of a 'short-range' scatterer.

a) Find the matrix element for scattering of electrons by all the point defects.

b) Assume the single-electron picture, and a parabolic bandstructure. Find an expression for the *momentum* scattering rate $1/\tau_m(E)$ of an electron due to the point defects as a function of its energy above the conduction band edge ($\epsilon = E - E_c$). Make necessary assumptions in the process. Show that the momentum and quantum scattering rates are the same for this form of isotropic scattering potentials.

c) Plot the mobility for 'thermal' electrons with $\epsilon = E - E_c \sim k_B T$ at 300 K, as a function of the impurity density in the range $n_{imp} = 10^{15} \to 10^{20}/\mathrm{cm}^3$ for various values of $V_0 = 0.1, 0.3, 0.5, 2.1$ eV. Assume an $R_0 \sim c/4$, where $c \sim 0.51$ nm is the c-axis lattice constant of GaN.

d) This is a reasonable model for things such as alloy scattering, for example, for charge transport of electrons in AlGaN and InGaN layers. Explain why an disordered alloy can be considered to be a perfect crystal with a high density of point defects. Then, estimate the mobility for electrons in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{N}$ layers as a function of the alloy composition x, by using your results in part (c). Find any references where this might have been done.

Solution:

Problem 4.5) Applications of Fermi's Golden Rule: Scattering rates due to point Defects.

(a).

$$M_{k'k} = \frac{1}{V}\int e^{i\vec{k}'\cdot\vec{r}}\, V_0\, \Theta(R_0 - |\vec{r}|)\, e^{-i\vec{k}\cdot\vec{r}}\, d\vec{r}$$

$$\vec{q} = \vec{k}' - \vec{k}.$$

$$M_{k'k} = \frac{2\pi V_0}{V}\int_0^{R_0} r^2 dr \cdot \int_{-1}^{1} e^{iqr\cos\theta}\, d(\cos\theta).$$

$$= \frac{2\pi V_0}{V}\int_0^{R_0} r^2 dr \cdot \frac{2\sin(qr)}{qr}$$

$$= \frac{4\pi V_0}{V}\cdot\frac{1}{q}\int_0^{R_0} r\sin(qr)\, dr$$

$$\boxed{M_{k'k} = \frac{4\pi V_0}{V}\cdot\frac{-qR_0\cos(qR_0)+\sin(qR_0)}{q^3}}$$

(b). $$S_{k\to k'} = \frac{2\pi}{\hbar}\cdot\left(\frac{4\pi V_0}{V}\right)^2\cdot\left[\frac{\sin(qR_0) - qR_0\cos(qR_0)}{q^3}\right]^2 \delta(E'-E)$$

$$q^2 = 2k^2(1-\cos\theta). \rightarrow \quad 1-\cos\theta = \frac{q^2}{2k^2}$$

$$d\cos\theta = \frac{q}{k^2}\, dq.$$

$$\frac{1}{\tau_k} = \sum_{\vec{k}'} S(k\to k')(1-\cos\theta).$$

$$= \frac{2\pi}{\hbar}\left(\frac{4\pi V_0}{V}\right)^2\cdot n_{imp} V\cdot\frac{V}{8\pi^3}\cdot 2\pi\int\left[\frac{\sin(qR_0) - qR_0\cos(qR_0)}{q^3}\right]^2 (1-\cos\theta)$$

$$k'^2\, dk'\, d\cos\theta \times \delta(E'-E)$$

$$k'^2 dk' = \frac{\sqrt{2m^* E}\; m^*}{\hbar^3}\, dE.$$

$$\frac{1}{\tau_k} = \frac{4\pi V_0^2 n_{imp}(2m^*)^{3/2} E^{1/2}}{\hbar^4}\int\left[\frac{\sin(qR_0) - qR_0\cos(qR_0)}{q^3}\right]^2 (1-\cos\theta)\, d\cos\theta$$

$$= 2\pi V_0^2 n_{imp}\left(\sqrt{2m^*}\right)^{-1} E^{-3/2}\int_0^{2k}\frac{[\sin(qR_0) - qR_0\cos(qR_0)]^2}{q^3}\, dq$$

$$= \frac{4\pi V_0^2 n_{imp} R_0^2}{\hbar^3 k^3}\int_0^{2kR_0}\frac{[\sin(x) - x\cos(x)]^2}{x^3}\, dx$$

(d). References:

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Problem 3.4: Flash Memory Design by Fermi's Golden Rule

Problem 3.4) Flash Memory Design by Fermi's golden rule

Figure 1 shows a 1-dimensional potential for an electron, which is in the state with energy E_0 at $t = 0$. Since there is a lower potential for $x > L_w + L_b$, the state $|E_0\rangle$ is a *quasi-bound* state. The electron is destined to leak out.

(a) Using WKB tunneling probability, and combining semi-classical arguments, find an analytical formula that estimates the time it takes for the electron to leak out. Find a value of this lifetime for $L_b \sim 3$ nm, $L_w \sim 2$ nm, $V_0 \sim 1$ eV, $E_0 \sim 2$ eV, and $E_b \sim 5$ eV. How many years does it take?

(b) This feature is at the heart of *flash memory*, which you use in computers and cell phones. Find an analytical expression that describes how the lifetime changes if a voltage V_a is applied across the insulator. Estimate the new lifetime for $V_a \sim 2.8$ V. This is the *readout* of the memory.

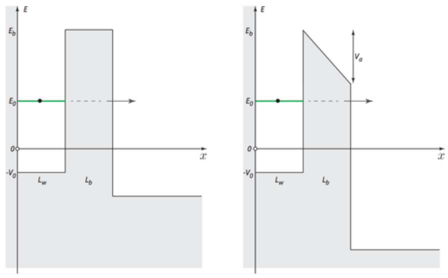


Figure 1: Escape and field-emission by tunneling.

(c) In the last two parts you invoked semi-classical arguments to estimate the tunneling escape time there. Now try solving the *same* problem using Fermi's golden rule. Model the problem carefully so that you can apply Fermi's golden rule. Discuss your approximations and their validity.

Solution:

(a)

a) Tunneling probability $T(E) = \exp - \int_0^{L_b} 2\, dx \sqrt{\frac{2m}{\hbar^2}(E_b - E_0)}$

$$= \exp\left(-2 L_b \sqrt{\frac{2m}{\hbar^2}(E_b - E_0)}\right)$$

A particle of energy E_0 in the region L_w has velocity $\sqrt{2(E_0+V_0)/m}$
It hits the right wall with a period $2L_w / \sqrt{2(E_0+V_0)/m}$. Each time it hits, the electron can tunnel out with probability $T(E_0)$.
The timescale to escape $\sim \frac{2L_w}{\sqrt{2(E_0+V_0)/m}} \cdot \frac{1}{T(E_0)}$

$$\simeq 20 \text{ years.}$$

(b)

(b) $T = \exp\left\{-2\int_0^{L_b} dx \sqrt{\frac{2m}{\hbar^2}\left(E_b - E_0 - q\frac{V_a x}{L_b}\right)}\right\}$

$= \exp\left\{-\frac{4L_b}{3qV_a}\frac{\sqrt{2m}}{\hbar}\left[(E_b - E_0)^{3/2} - (E_b - E_0 - qV_a)^{3/2}\right]\right\}$

lifetime ~ 81 second.

(C)

(a) WKB result.

$$\tau_{WKB} \sim 2L_w\sqrt{\frac{m}{2(E_0+V_0)}}\ \exp\left[2\sqrt{\frac{2m}{\hbar^2}(E_b-E_0)}\ L_b\right]$$

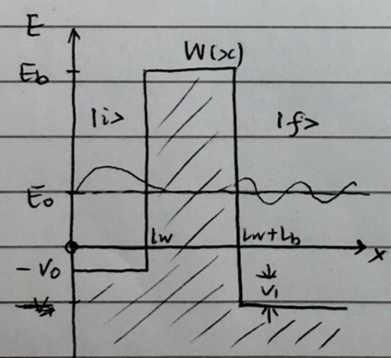
No bias $\quad \tau_{WKB} \sim 4.7\times10^8\ s \quad \sim 15$ years

With bias $\quad \tau_{WKB} \sim 62\ s \quad \sim 1$ min,

(b) Fermi's golden rule.

$$\frac{1}{\tau_{i\to f}} = \frac{2\pi}{\hbar}\,|\underbrace{\langle\psi_f|W(x)|\psi_i\rangle}_{M_{fi}:\ \text{Matrix element.}}|^2\ \delta(E_f-E_i)$$

(1). No bias. $\qquad W(x)=E_b$.



$\boxed{\text{initial state}}$

$$\psi_i(x)=\begin{cases}A\sin(k_0x) & 0\le x\le L_w\\ B\exp[-k_b(x-L_w)] & x\ge L_w\end{cases}$$

where $k_0=\sqrt{\frac{2m}{\hbar^2}(E_0+V_0)}$

$k_b=\sqrt{\frac{2m}{\hbar^2}(E_b-E_0)}$

Continuities of ψ_i and ψ_i' at $x=L_w$ gives $\quad A^2=B^2\cdot\frac{E_b+V_0}{E_0+V_0}$

Normalization of ψ_i requires.

$$B^2=\left\{\frac{1}{2k_b}-\frac{E_b+V_0}{E_0+V_0}\left[\frac{\sin(2k_0L_w)}{4k_0}-\frac{L_w}{2}\right]\right\}^{-1}$$

For the given parameters

$$B\sim\sqrt{\frac{E_0+V_0}{E_b+V_0}\cdot\frac{2}{L_w}}$$

$\Rightarrow$ Initial state inside the barrier:

$$\psi_i(x)=\sqrt{\frac{E_0+V_0}{E_b+V_0}\cdot\frac{2}{L_w}}\ e^{-k_b(x-L_w)}$$

$\boxed{\text{final state}}$

assume a wall exists at $L_R \to \infty$ to reflect the electron.

$$\psi_f(x) = \begin{cases} C e^{ik_r x} + D e^{-ik_r x} & L_w + L_b \le x \le L_R \\ F e^{k_b[x-(L_w+L_b)]} & x \geqslant L_w + L_b \end{cases}$$

where $k_r = \sqrt{\frac{2m}{\hbar^2}(E_0+V_0+V_1)}$

continuity and normalization of $\psi_f(x) \Rightarrow F = \sqrt{\frac{E_0+V_0+V_1}{E_b+V_0+V_1} \cdot \frac{2}{L_R}}$

$\Rightarrow$ final state inside the barrier:

$$\psi_f(x) = \sqrt{\frac{E_0+V_0+V_1}{E_b+V_0+V_1} \cdot \frac{2}{L_R}} \, e^{k_b[x-(L_w+L_b)]}$$

$\boxed{\text{Matrix element}}$

$$M_{fi} = E_b \sqrt{\frac{E_0+V_0+V_1}{E_b+V_0+V_1} \frac{E_0+V_0}{E_b+V_0}} \sqrt{\frac{2}{L_R} \frac{2}{L_w}} \int_{L_w}^{L_w+L_b} e^{-k_b L_b} \, dx$$

assume $V_1 \ll E_0 + V_0$.

$$M_{fi} = E_b L_b \left(\frac{E_0+V_0}{E_b+V_0}\right) \sqrt{\frac{4}{L_R L_W}} \, e^{-k_b L_b}.$$

$$|M_{fi}|^2 = E_b^2 L_b^2 \left(\frac{E_0+V_0}{E_b+V_0}\right)^2 \frac{4}{L_R L_W} e^{-2k_b L_b}$$

$\boxed{\text{Transion rate}}$

$$\frac{1}{\tau_{i \to f}} = \frac{2\pi}{\hbar} E_b^2 L_b^2 \left(\frac{E_0+V_0}{E_b+V_0}\right)^2 \frac{4}{L_R L_W} e^{-2k_b L_b} \delta(E_f - E_i)$$

$\boxed{\text{Escape rate}}$ $\quad \frac{1}{\tau_{FGR}} = \sum_{k_f} \frac{1}{\tau_{i \to f}} = \int dE_f \, g(E_f) \frac{1}{\tau_{i \to f}}$

Density of states: $g(E_f) = \frac{2L_R}{\pi} \sqrt{\frac{m}{2\hbar^2 E_f}}$

$\cdot \; E_f = E_i = E_0 + V_0$

$$\frac{1}{\tau_{FGR}} = 8 \sqrt{\frac{2m}{E_0+V_0}} \frac{1}{\hbar^2} \frac{L_b^2}{L_W} E_b^2 \left(\frac{E_0+V_0}{E_b+V_0}\right)^2 e^{-2k_b L_b}.$$

②

Escape time:

$$\tau_{FGR} = \frac{\hbar^2}{8}\sqrt{\frac{E_0+V_0}{2m}}\;\frac{L_w}{L_b^2}\;\frac{1}{E_b^2}\left(\frac{E_b+V_0}{E_0+V_0}\right)^2 e^{2k_b L_b}.$$

Compare with WKB results.

$$\tau_{WKB} = 2L_w\sqrt{\frac{m}{2(E_0+V_0)}}\; e^{2k_b L_b}.$$

$$\frac{\tau_{FGR}}{\tau_{WKB}} \sim \frac{\hbar^2}{16 m L_b^2 (E_0+V_0)} \sim 0.00018$$

(2) With bias.

$$E_b \to E_b - \frac{eV_a}{L_b}(x-L_w)$$

and do the similar calculation. as in no bias case

Problem 3.5: Higher-order time-dependent perturbation theory: Dyson series and diagrams

Problem 3.5) Higher-order time-dependent perturbation theory: Dyson series and diagrams

In class, we used the *interaction representation* to write the perturbed quantum state at time t as $|\psi_t\rangle = e^{-i\frac{H_0}{\hbar}t}|\psi(t)\rangle$, where H_0 is the unperturbed Hamiltonian *operator*. This step helped us recast the time-dependent Schrodinger equation $i\hbar\frac{\partial}{\partial t}|\psi_t\rangle = (H_0 + W_t)|\psi_t\rangle$ to the simpler form $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = W(t)|\psi(t)\rangle$, where $W(t) = e^{+i\frac{H_0}{\hbar}t}W_t e^{-i\frac{H_0}{\hbar}t}$ is the time-evolution operator. This equation was integrated over time to yield the Dyson series

$$\begin{aligned}|\psi(t)\rangle = \underbrace{|0\rangle}_{|\psi(t)\rangle^{(0)}} &+ \underbrace{\frac{1}{i\hbar}\int_{t_0}^{t} dt' W(t')|0\rangle}_{|\psi(t)\rangle^{(1)}} + \underbrace{\frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' W(t')W(t'')|0\rangle}_{|\psi(t)\rangle^{(2)}} \\ &+ \underbrace{\frac{1}{(i\hbar)^3}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt''' W(t')W(t'')W(t''')|0\rangle}_{|\psi(t)\rangle^{(3)}} + ..., \end{aligned} \tag{5}$$

where $|\psi(t_0)\rangle = |0\rangle$ is the initial state. Restricting the Dyson series to the 1st order term in W for a perturbation of the the form $W_t = e^{\eta t}W(r)$, we derived Fermi's golden rule for the transition rate $\Gamma^{(1)}_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W(r)|0\rangle|^2\delta(\epsilon_0 - \epsilon_n)$. We used the relation $\lim_{\eta\to 0^+}\frac{2\eta}{x^2+\eta^2} = 2\pi\delta(x)$ in this process.

a) Show that the second and third order terms in W in the Dyson series lead to a modified golden rule result

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W|0\rangle + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{\epsilon_0 - \epsilon_m + i\eta\hbar} + \sum_{k,l}\frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|V|0\rangle}{(\epsilon_0 - \epsilon_k + 2i\eta\hbar)(\epsilon_0 - \epsilon_l + i\eta\hbar)} + ...|^2\delta(\epsilon_0 - \epsilon_n), \tag{6}$$

where in the end we take $\eta \to 0^+$. We identify the Green's function propagators of the form $G = \sum_m \frac{|m\rangle\langle m|}{\epsilon_0 - \epsilon_m + i\eta\hbar}$. Thus, the result to higher orders may be written in the compact form

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar}|\langle n|W + WGW + WGWGW + ...|0\rangle|^2\delta(\epsilon_0 - \epsilon_n). \tag{7}$$

5.23 A one-dimensional harmonic oscillator is in its ground state for $t < 0$. For $t \geq 0$ it is subjected to a time-dependent but spatially uniform *force* (not potential!) in the x-direction,

$$F(t) = F_0 e^{-t/\tau}.$$

(a) Using time-dependent perturbation theory to first order, obtain the probability of finding the oscillator in its first excited state for $t > 0$. Show that the $t \to \infty$ (τ finite) limit of your expression is independent of time. Is this reasonable or surprising?

(b) Can we find higher excited states? You may use

$$\langle n'|x|n\rangle = \sqrt{\hbar/2m\omega}(\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}).$$

Figure 2: Harmonic oscillator perturbed by a time-dependent field.

b) Sketch the 'Feynman' diagrams[1] corresponding to the terms in the series, showing the *virtual* states explicitly for the higher order terms.

c) Solve the above problem in Figure 2 from Sakurai (Modern Quantum Mechanics). Note that for part (b), you will need to invoke higher-order perturbation terms as discussed in this problem, the 1st order Fermi's golden rule result term will not be enough.

[1]More accurately, Goldstone diagrams.

Solution:

(a,b)

Problem 4.2) Higher-order time-dependent perturbation theory: Dyson series and diagrams.

(a):

$$|\psi(t)\rangle^{(1)} = \frac{1}{i\hbar}\int_{t_0}^{t} dt'\, W(t')\,|0\rangle$$

$$|\psi(t)\rangle^{(2)} = \frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, W(t')\,W(t'')\,|0\rangle$$

$$|\psi(t)\rangle^{(3)} = \frac{1}{(i\hbar)^3}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \int_{t_0}^{t''} dt'''\, W(t')\,W(t'')\,W(t''')\,|0\rangle$$

$$W(t) = e^{i\frac{H_0}{\hbar}t}\, W_t\, e^{-i\frac{H_0}{\hbar}t} = e^{i\frac{H_0}{\hbar}t}\, e^{\eta t}\, W\, e^{-i\frac{H_0}{\hbar}t}$$

(1). $$\langle n|\psi(t)\rangle^{(2)} = \frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \langle n| e^{i\frac{H_0}{\hbar}t'} e^{\eta t'}\, W e^{-i\frac{H_0}{\hbar}t'}\, e^{i\frac{H_0}{\hbar}t''} e^{\eta t''}\, W e^{-i\frac{H_0}{\hbar}t''} |0\rangle$$

insert virtual states.

$$\langle n|\psi(t)\rangle^{(2)}$$

$$= \sum_m \frac{1}{(i\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, \langle n| e^{i\frac{H_0}{\hbar}t'} e^{\eta t'}\, W e^{-i\frac{H_0}{\hbar}t'} |m\rangle\langle m| e^{i\frac{H_0}{\hbar}t''} e^{\eta t''}\, W e^{-i\frac{H_0}{\hbar}t''} |0\rangle$$

$$= \frac{1}{(i\hbar)^2}\sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t''} dt''\, e^{i\frac{E_n-E_m}{\hbar}t'}\, e^{\eta t'} \langle n|W|m\rangle\, e^{i\frac{E_m-E_0}{\hbar}t''}\, e^{\eta t''} \langle m|W|0\rangle$$

$$= \frac{1}{(i\hbar)^2}\sum_m \langle n|W|m\rangle\langle m|W|0\rangle \int_{t_0}^{t} dt'\, e^{i\frac{E_n-E_m}{\hbar}t'}\, e^{\eta t'} \left\{ \frac{e^{i\frac{E_m-E_0}{\hbar}t'} e^{\eta t'} - e^{i\frac{E_m-E_0}{\hbar}t_0} e^{\eta t_0}}{i\left(\frac{E_m-E_0}{\hbar}\right)+\eta} \right\}$$

set $t_0 \to -\infty$. $\because \eta \to 0^+$. $e^{\eta t_0} \to 0$.

$$\langle n|\psi(t)\rangle^{(2)} = \frac{1}{(i\hbar)^2}\sum_m \langle n|W|m\rangle\langle m|W|0\rangle . \int_{t_0}^{t} dt'\, e^{i\frac{E_n-E_0}{\hbar}t'}\, e^{2\eta t'} \frac{1}{i\left(\frac{E_m-E_0}{\hbar}\right)+\eta}$$

$$= \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{E_0-E_m+i\eta\hbar} \cdot \frac{e^{i\frac{E_n-E_0}{\hbar}t}\, e^{2\eta t}}{E_0-E_n+2i\eta\hbar}$$

Similarly.

(2) $$\langle n|\psi(t)\rangle^{(3)} = \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|W|0\rangle}{(E_0-E_k+2i\eta\hbar)(E_0-E_l+i\eta\hbar)} \cdot \frac{e^{i\frac{E_n-E_0}{\hbar}t}\, e^{3\eta t}}{E_0-E_n+3i\eta\hbar}$$

(3)

$$\langle n | \psi(t) \rangle^{(1)+(2)+(3)}$$

$$= \langle n|W|0\rangle \frac{e^{i\frac{E_n-E_0}{\hbar}t} e^{\eta t}}{E_0 - E_n + i\eta\hbar} + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{E_0 - E_m + i\eta t} \cdot \frac{e^{i\frac{E_n-E_0}{\hbar}t} e^{\eta t}}{E_0 - E_n + 2i\eta\hbar}$$

$$+ \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|W|0\rangle}{(E_0 - E_k + 2i\eta\hbar)(E_0 - E_l + i\eta\hbar)} \frac{e^{i\frac{E_n-E_0}{\hbar}t} e^{\eta t}}{E_0 - E_n + 3i\eta\hbar}$$

when $\eta \to 0^+$. $\eta \sim 2\eta \sim 3\eta$.

$$|\langle n|\psi(t)\rangle|^2$$

$$= \left| \langle n|W|0\rangle + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{E_0 - E_m + i\eta\hbar} + \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|W|0\rangle}{(E_0 - E_k + 2i\eta\hbar)(E_0 - E_l + i\eta\hbar)} \right|^2$$

$$\times \left| \frac{e^{\eta t}}{E_0 - E_n + i\eta\hbar} \right|^2$$

$$\frac{\partial}{\partial t} \left| \frac{e^{\eta t}}{E_0 - E_n + i\eta\hbar} \right|^2 = \frac{\partial}{\partial t} \left[\frac{2\eta}{(E_0 - E_n)^2 + (\eta\hbar)^2} \right] = \frac{2\pi}{\hbar} \delta(E_0 - E_n)$$

$\Rightarrow$ higher order golden rule.

$$\Gamma_{0\to n} = \frac{\partial}{\partial t} |\langle n|\psi(t)\rangle|^2$$

$$= \frac{2\pi}{\hbar} \left| \langle n|W|0\rangle + \sum_m \frac{\langle n|W|m\rangle\langle m|W|0\rangle}{E_0 - E_m + i\eta\hbar} + \sum_{k,l} \frac{\langle n|W|k\rangle\langle k|W|l\rangle\langle l|W|0\rangle}{(E_0 - E_k + 2i\eta\hbar)(E_0 - E_l + i\eta\hbar)} \right|^2 \delta(E_0 - E_n)$$

$$\Gamma_{0\to n} = \frac{2\pi}{\hbar} |\langle n| W + WGW + WGWGW + \dots |0\rangle|^2 \delta(E_0 - E_n)$$

(C)

Problem 4.3) Application of 1st and higher order perturbation theories.

(a). Perturbation potential.

$$V(x) = \int_0^x F(t) = F_0 e^{-t/\tau} = F_0 x e^{-t/\tau} \qquad (t \geq 0)$$

(Let $V(0) = 0$).

$$\langle n | \psi(t) \rangle^{(1)} = \langle n | 0 \rangle + \frac{1}{i\hbar} \int_0^t dt' \langle n | e^{i \frac{H_0}{\hbar} t'} e^{-t'/\tau} F_0 x e^{-\frac{H_0}{\hbar} t'} | 0 \rangle$$

$$= \frac{1}{i\hbar} F_0 \langle n | x | 0 \rangle \int_0^t dt' \, e^{i \frac{E_n - E_0}{\hbar} t'} e^{-t'/\tau}$$

$$= F_0 \langle n | x | 0 \rangle \frac{e^{i \frac{E_n - E_0}{\hbar} t} e^{-t/\tau} - 1}{E_0 - E_n - i\hbar/\tau}$$

for first excited state

$$\langle 1 | x | 0 \rangle = \sqrt{\hbar / 2m\omega}$$

$$\langle 1 | \psi(t) \rangle^{(1)} = F_0 \sqrt{\hbar / 2m\omega} \cdot \frac{e^{i \frac{E_1 - E_0}{\hbar} t} e^{-t/\tau} - 1}{E_0 - E_1 - i\hbar/\tau}$$

$$| \langle 1 | \psi(t) \rangle^{(1)} |^2 = \frac{\hbar}{2m\omega} F_0^2 \frac{e^{-2t/\tau} - 2e^{-t/\tau} \cos\left(\frac{E_1 - E_0}{\hbar} t\right) + 1}{(E_0 - E_1)^2 + \hbar^2/\tau^2}$$

$E_n = (n + \frac{1}{2}) \hbar\omega$, $E_0 = \frac{1}{2}\hbar\omega$, $E_1 = \frac{3}{2}\hbar\omega$, $E_1 - E_0 = \hbar\omega$

$$| \langle 1 | \psi(t) \rangle^{(1)} |^2 = \frac{\hbar}{2m\omega} F_0^2 \frac{e^{-2t/\tau} - 2e^{-t/\tau} \cos(\omega t) + 1}{\hbar^2\omega^2 + \hbar^2/\tau^2}$$

$$= \frac{F_0^2}{2m\hbar\omega} \frac{e^{-2t/\tau} - 2e^{-t/\tau} \cos(\omega t) + 1}{\omega^2 + 1/\tau^2}$$

$t \to \infty \qquad e^{-t/\tau} \to 0$

$$| \langle 1 | \psi(t) \rangle^{(1)} |^2 \Big|_{t \to \infty} = \frac{F_0^2}{2m\hbar\omega} \frac{\tau^2}{\omega^2 \tau^2 + 1}$$

$\to$ approaching steady state.

(b) higher $(n \geq 2)$ excited states

$\because$ when $n \geq 2$ $\quad \langle n | x | 0 \rangle = 0$

$\Rightarrow \quad \langle n | \psi(t) \rangle^{(1)} = 0.$

$\Rightarrow$ higher order terms need to be considered.

$$\langle 2 | \psi(t) \rangle^{(2)} = \frac{F_0^2}{(i\hbar)^2} \sum_m \langle 2 | x | m \rangle \langle m | x | 0 \rangle \int_0^t dt' \, e^{i \frac{E_2 - E_m}{\hbar} t'} e^{-t'/\tau} \left\{ \frac{e^{i \frac{E_m - E_0}{\hbar} t'} e^{-t'/\tau} - 1}{i \left(\frac{E_m - E_0}{\hbar} \right) - 1/\tau} \right\}$$

only $m=1$ term is non-zero.

$$\langle 2 | \psi(t) \rangle^{(2)} = \frac{F_0^2}{(i\hbar)^2} \cdot \frac{\hbar}{\sqrt{2} m\omega} \frac{1}{(i\omega - \frac{1}{\tau})} \int_0^t dt' \left[e^{2i\omega t' - 2t'/\tau} - e^{i\omega t' - t'/\tau} \right]$$

$$= \frac{F_0^2}{(i\hbar)^2} \cdot \frac{\hbar}{\sqrt{2} m\omega} \frac{1}{i\omega - \frac{1}{\tau}} \left[\frac{e^{2i\omega t - 2t/\tau} - 1}{2(i\omega - \frac{1}{\tau})} - \frac{e^{i\omega t - t/\tau} - 1}{(i\omega - \frac{1}{\tau})} \right]$$

$$= \frac{F_0^2}{(i\hbar)^2} \frac{\hbar}{\sqrt{2} m\omega} \cdot \frac{1}{2(i\omega - \frac{1}{\tau})^2} \cdot \left(e^{i\omega t - t/\tau} - 1 \right)^2$$

$$= \frac{F_0^2}{2\sqrt{2} m \hbar \omega (\omega + i \frac{1}{\tau})^2} \left(e^{i\omega t - t/\tau} - 1 \right)^2$$

$$| \langle 2 | \psi(t) \rangle^{(2)} |^2 = \frac{F_0^4 \tau^4}{8 m^2 (\hbar\omega)^2 (\omega^2 \tau^2 + 1)^2} \left| \left(e^{i\omega t - t/\tau} - 1 \right)^2 \right|^2$$

$$= \frac{F_0^4 \tau^4}{8 m^2 (\hbar\omega)^2 (\omega^2 \tau^2 + 1)^2} \Big[e^{-4t/\tau} - 4\cos(\omega t) e^{-3t/\tau} + 2\cos(2\omega t) e^{-2t/\tau} - 4\cos(\omega t) e^{-t/\tau} + 1 \Big]$$

Problem 3.6: Prelim: Electron Mobility in Semiconductors

Problem 3.6) Prelim: Electron Mobility in Semiconductors

The purpose of this question is to reproduce the theoretical calculation of electron mobility vs temperature as shown in Figure 3 and explain the physics of electron transport underlying what is measured in the experiment. This requires you to calculate the scattering rates due to phonons, ionized impurities, and neutral impurities, and applying the Boltzmann transport equation to evaluate the electron mobility vs temperature. On the class website I have provided you with a handout from Wolfe / Holonyak / Stillman to help you in this problem, and the paper from where this plot is taken, so you have everything you need to solve this problem.

(a) Boltzmann Transport Equation We derived the solution to the Boltzmann transport equation in the relaxation-time approximation for elastic scattering events to be $f(\mathbf{k}) \approx f_0(\mathbf{k}) + \tau(\mathbf{k})(-\frac{\partial f_0(\mathbf{k})}{\partial \mathcal{E}(\mathbf{k})})\mathbf{v_k} \cdot \mathbf{F}$, where all symbols have their usual meanings. Use this to show that for transport in d dimensions in response to a constant electric field E, in a semiconductor with an isotropic effective mass $m^\star$, the current density is $J = \frac{nq^2\langle\tau\rangle}{m^\star}E$, where $\langle\tau\rangle = \frac{2}{d} \cdot \frac{\int d\mathcal{E} \cdot \tau(\mathcal{E})\mathcal{E}^{\frac{d}{2}}(-\frac{\partial f_0(\mathcal{E})}{\partial \mathcal{E}})}{\int d\mathcal{E} \cdot \mathcal{E}^{\frac{d}{2}-1} f_0(\mathcal{E})}$, where the integration variable $\mathcal{E} = \mathcal{E}(\mathbf{k})$ is the kinetic energy of carriers. $\mu = \frac{q\langle\tau\rangle}{m^\star}$ is the mobility. You have now at your disposal the *most general form* of conductivity and mobility from the Boltzmann equation for semiconductors that have a parabolic bandstructure! *Hint:* You may need the result that the volume of a d-dimensional sphere in the k-space is $V_d = \frac{\pi^{\frac{d}{2}} k^d}{\Gamma(\frac{d}{2}+1)}$, and some more dimensional and $\Gamma-$function information.

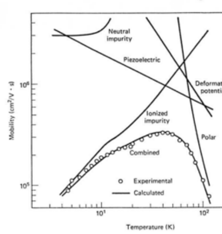


Figure 6.7 Temperature dependence of the mobility for *n*-type GaAs showing the separate and combined scattering processes. [From C. M. Wolfe, G. E. Stillman, and W. T. Lindley, *J. Appl. Phys. 41*, 3088 (1970).]

Figure 3: Electron mobility in doped GaAs semiconductor at high temperatures is limited by phonon scattering, and by impurity and defect scattering at low temperatures. In this problem, you will calculate the solid lines of this plot.

(b) Spatially uncorrelated scattering points: Show using Fermi's golden rule that if the scattering rate of electrons in a band of a semiconductor due to the presence of ONE scatterer of potential $W(r)$ centered at the origin is $S(\mathbf{k} \to \mathbf{k'}) = \frac{2\pi}{\hbar}|\langle\mathbf{k'}|W(r)|\mathbf{k}\rangle|^2\delta(E_{\mathbf{k}} - E_{\mathbf{k'}})$, then the scattering rate due to N_s scatterers distributed *randomly and uncorrelated* in 3D space is $N_s \cdot S(\mathbf{k} \to \mathbf{k'})$. In other words, the scattering rate increases *linearly* with the number of uncorrelated scatterers, which implies that the mobility limited by such scattering will decrease as $1/N_s$. This argument is subtle, and effects of electron wave interference should enter your analysis. [*Hint*: Add the potentials of each randomly distributed impurity for the total potential $W_{tot}(r) = \sum_i W(\mathbf{r} - \mathbf{R_i})$. Use the effective mass equation for the electron states to show that the matrix element is a Fourier transform. Then invoke the shifting property of Fourier transforms.] Now calculate the neutral impurity scattering limited mobility for GaAs and compare with Figure 3.

(c) Impurity scattering: Using Fermi's golden rule, calculate the scattering rate for electrons due to a screened Coulombic charged impurity potential $V(r) = -\frac{Ze^2}{4\pi\epsilon_s r}e^{-\frac{r}{L_D}}$, where Ze is the charge of the impurity, ϵ_s is the dielectric constant of the semiconductor, and $L_D = \sqrt{\frac{\epsilon_s k_b T}{ne^2}}$ is the Debye screening length and n is the free carrier density. This is the scattering rate for just one impurity. Show using the result in parts (a) and (b), with a $1 - \cos\theta$ angular factor for mobility that if the charged-impurity density is N_D, the mobility for 3D carriers is $\mu_I = \frac{2^{\frac{7}{2}}(4\pi\epsilon_s)^2(k_b T)^{\frac{3}{2}}}{\pi^{\frac{3}{2}} Z^2 e^3 \sqrt{m^\star} N_D F(\beta)} \sim \frac{T^{\frac{3}{2}}}{N_D}$. Here $\beta = 2\sqrt{\frac{2m^\star(3k_b T)}{\hbar^2}}L_D$ is a dimensionless parameter, and $F(\beta) = \ln[1+\beta^2] - \frac{\beta^2}{1+\beta^2}$ is a weakly varying function. This famous result is named after Brooks and Herring who derived it first. Calculate the ionized impurity scattering limited mobility and compare: are your values close to what is experimentally observed for these conditions as shown in Figure 3?

(d) Acoustic Phonon scattering: The scattering rate of electrons due to acoustic phonons in semiconductors is given by Fermis golden rule result for time-dependent oscillating perturbations $\frac{1}{\tau(\mathbf{k}\to\mathbf{k'})} = \frac{2\pi}{\hbar}|\langle\mathbf{k'}|W(\mathbf{r})|\mathbf{k}\rangle|^2\delta(E_{\mathbf{k}} - E_{\mathbf{k'}} \pm \hbar\omega_q)$, where the acoustic phonon dispersion for low energy (or long wavelength) is $\omega_q \sim v_s q$ with v_s the sound velocity, and the scattering potential is $W(\mathbf{r}) = D_c \nabla_{\mathbf{r}} \cdot \mathbf{u}(\mathbf{r})$. Here D_c is the deformation potential (units: eV), and $\mathbf{u}(\mathbf{r}) = \hat{\mathbf{n}} u_0 e^{i\mathbf{q}\cdot\mathbf{r}}$ is the spatial part of the phonon displacement wave, $\hat{\mathbf{n}}$ is the unit vector in the direction of atomic vibration, and the phonon wavevector $\mathbf{q}$ points in the direction of the phonon wave propagation. We also justified why the amplitude of vibration u_0 may be found from $2M\omega_q^2 u_0^2 \approx N_{ph} \times \hbar\omega_q$, where $N_{ph} = 1/[e^{\frac{\hbar\omega_q}{k_b T}} - 1]$ is the Bose-number of phonons, and the mass of a unit cell of volume Ω is $M = \rho\Omega$, where ρ is the mass density (units: kg.m^{-3}). Show that a transverse acoustic (TA) phonon does *not* scatter electrons, but longitudinal acoustic (LA) phonons do. By evaluating the scattering rate using Fermi's golden rule, and using the the ensemble averaging of Problem 25 (a), show that the electron mobility in three dimensions due to LA phonon scattering is $\mu_{LA} = \frac{2\sqrt{2\pi}}{3}\frac{q\hbar^4\rho v_s^2}{(m_c^\star)^{\frac{5}{2}} D_c^2 (k_b T)^{\frac{3}{2}}} \sim T^{-\frac{3}{2}}$. This is a *very* useful result. Calculate and explain the acoustic deformation potential and acoustic piezoelectric phonon scattering rates for GaAs and compare with Figure 3.

(e) Discuss how polar optical phonon scattering is different from acoustic phonon scattering, and calculate the phonon scattering limited mobility for GaAs and compare with Figure 3.

(f) Now combine all the above parts of to explain the experimental dependence of mobility vs temperature and as a function of impurity density as seen in Figure 3. If you have succeeded in getting it to work, you have built a very powerful transport tool - because now you can use it to explain electron transport properties in *any* semiconductor! This is because the material parameters may change, but the transport formalism remains the same.

Solution:

(a) Boltzmann Transport Equation in d-dimensions

)·4)

$$f(k) \approx f_0(k) + \tau(k)\left(-\frac{\partial f_0(k)}{\partial E(k)}\right)\vec{v}_k\cdot\vec{F}$$

$\vec{F}$ ← force $= -q\vec{E}$ ← electric field.

$$\approx f_0(k) + q\tau(k)\left(+\frac{\partial f_0(k)}{\partial E(k)}\right)\cdot\vec{v}_k\cdot\vec{E}$$

Carrier density: $n = \frac{\overset{\text{spin}}{g_s}\,\overset{\text{valley}}{g_v}}{L^d}\sum_k f(k) = \frac{g_s g_v}{L^d}\cdot\int\frac{d^dk}{\left(\frac{2\pi}{L}\right)^d}\,f(k)$

$f(k) = \underbrace{f_0(k)}_{\text{even.}} + \underbrace{q\tau(k)\left(\frac{\partial f_0}{\partial E}\right)\vec{v}\cdot\vec{E}}_{\text{odd} \to 0!}$

$\Rightarrow$

$$n = \frac{g_s g_v}{(2\pi)^d}\int d^dk\; f_0(k)$$

Volume of a d-dimensional sphere in k-space: $\boxed{V_d = \frac{\pi^{d/2}k^d}{\Gamma(\frac{d}{2}+1)}}$ Check: $d=2 \Rightarrow \pi k^2$, $d=3 \Rightarrow \frac{4}{3}\pi k^3\ldots$

"Surface" of a d-dimensional sphere in k-space:

$$\boxed{S_d = \nabla_k V_d = \frac{d\,\pi^{d/2}k^{d-1}}{\Gamma(d/2+1)}}$$

Check: $d=2 \Rightarrow 2\pi k$, $d=3 \Rightarrow 4\pi k^2\ldots$

$\Rightarrow$ Carrier density in d-dimensions is:

$$n = \frac{g_s g_v}{(2\pi)^d}\int\frac{d\cdot\pi^{d/2}k^{d-1}\,dk}{\Gamma(\frac{d}{2}+1)}\cdot f_0(k)$$

$$E = E_c + \underbrace{\frac{\hbar^2k^2}{2m^*}}_{\varepsilon_k}$$

$$= \frac{g_s g_v\cdot d\cdot\pi^{d/2}}{(2\pi)^d\Gamma(\frac{d}{2}+1)}\int k^{d-1}dk\cdot f_0(k)$$

$$\Rightarrow k^{d-1}dk = \frac{2m^*}{2\cdot\hbar^2}\left\{\frac{2m^*}{\hbar^2}\underbrace{(E-E_c)}_{\varepsilon}\right\}^{\frac{d}{2}-1} dE$$

$$n = \frac{g_s g_v\, d\cdot\pi^{d/2}}{(2\pi)^d\Gamma(\frac{d}{2}+1)}\cdot\frac{1}{2}\cdot\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\int d\varepsilon\cdot\varepsilon^{\frac{d}{2}-1}f_0(\varepsilon)$$

$$\boxed{k^{d-1}dk = \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\varepsilon^{\frac{d}{2}-1}}$$

$$\boxed{n = \int g_d(\varepsilon)f_0(\varepsilon)d\varepsilon}, \text{ where } \boxed{g_d(\varepsilon) = \frac{g_s g_v}{2^{d-2}\pi^{d/2}\Gamma(\frac{d}{2})}\left(\frac{2m^*}{\hbar^2}\right)^{d/2}\varepsilon^{\frac{d}{2}-1}}$$

generalized d-dimensional DOS.

Similarly, $\vec{J} = q\cdot\frac{g_s g_v}{L^d}\sum_k f(k)\vec{v}_k$

Let the electric field point along a fixed direction $\vec{E}$, say $\hat{x}$.

Then, $f(\vec{k}) \simeq f_0(\vec{k}) + q\tau(\vec{k})\left(+\frac{\partial f_0}{\partial\varepsilon_k}\right)\vec{v}_k\cdot\vec{E}$

$$\Rightarrow \vec{J} = q\cdot\frac{g_s g_v}{L^d}\int\frac{d^dk}{\left(\frac{2\pi}{L}\right)^d}\vec{v}_k\cdot\left[\cancelto{0}{f_0(\vec{k})} + q\tau(\vec{k})\left(-\frac{\partial f_0(\vec{k})}{\partial\varepsilon_k}\right)\cdot\vec{v}_k\cdot\vec{E}\right]$$

$$= q^2\frac{g_s g_v}{(2\pi)^d}\int d^dk\;\underbrace{\vec{v}_k(\vec{v}_k\cdot\vec{E})}_{?}\cdot\tau(\vec{k})\left(-\frac{\partial f_0(\vec{k})}{\partial\varepsilon_k}\right)$$

Now $\vec{v}_k(\vec{v}_k\cdot\vec{E}) = \vec{v}_k v_{kx}E = \vec{v}_k v_k\cos\theta_k E$

&

$$J_x = \left\{q^2\cdot\frac{g_s g_v}{(2\pi)^d}\cdot\int d^dk\; v_k^2\cos^2\theta_k\,\tau(\vec{k})\left(-\frac{\partial f_0(\vec{k})}{\partial\varepsilon_k}\right)\right\} * E$$

$$\frac{J_x}{n} = q^2\frac{\int d_kV_d\; v_k^2\cos^2\theta_k\,\tau(\vec{k})\left(-\frac{\partial f_0}{\partial\varepsilon_k}\right)}{\int d_kV_d\cdot f_0(\vec{k})}$$

$v_k^2 = \frac{2\varepsilon_k}{m^*}$

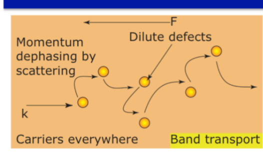
$\boxed{\langle\cos^2\theta_k\rangle = \frac{1}{d}}$ ← Note!

$$\Rightarrow J_x = \frac{n\cdot q^2}{m^*}\left\{\frac{2}{d}\cdot\frac{\int d\varepsilon_k\,\varepsilon_k^{d/2}\tau(\varepsilon_k)\left(-\frac{\partial f_0}{\partial\varepsilon_k}\right)}{\int d\varepsilon_k\cdot\varepsilon_k^{d/2-1}f_0(\varepsilon_k)}\right\}$$

$$\Rightarrow \boxed{J_x = \frac{n\cdot q^2}{m^*}\langle\tau\rangle}$$

(b) Spatially uncorrelated scattering points

Transport in the 'Diffusive' Limit



$$\frac{1}{\tau_{\mathbf{kk'}}} = \frac{2\pi}{\hbar}|V(\mathbf{q})|^2\delta[E_{\mathbf{k'}} - (E_{\mathbf{k}} \pm \hbar\omega)]$$

$$\mathbf{q} = \mathbf{k} - \mathbf{k'}$$

$$V(\mathbf{q}) = \langle\mathbf{k'}|W(\mathbf{r})|\mathbf{k}\rangle$$

Fermi's Golden Rule tells us that the scattering potential is the SUM of ALL the scatterers in the macroscopic crystal.

How do multiple scattering centers add up and contribute to the total scattering rate?

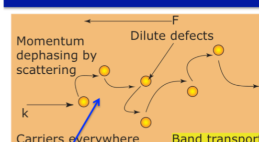
$$= \int_V\left[\frac{e^{-i\mathbf{k'}\cdot\mathbf{r}}}{\sqrt{V}}u^\star_{\mathbf{K}}(\mathbf{r})\right]\times W(\mathbf{r})\times\left[\frac{e^{+i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}}u_{\mathbf{K}}(\mathbf{r})\right]d^3\mathbf{r}$$

$$= \int_V\left[\frac{e^{i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{r}}}{V}\right]W(\mathbf{r})\times[u^\star_{\mathbf{K}}(\mathbf{r})u_{\mathbf{K}}(\mathbf{r})]d^3\mathbf{r}$$

$$\approx \underbrace{\left(\int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r})\frac{d^3\mathbf{r}}{V}\right)}_{crystal}\times\underbrace{\left(\int_\Omega u^\star_{\mathbf{K}}(\mathbf{r})u_{\mathbf{K}}(\mathbf{r})\frac{d^3\mathbf{r}}{\Omega}\right)}_{=1}$$

Fourier Transform of real-space scattering potential! $\boxed{V(\mathbf{q}) \approx \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r})\frac{d^3\mathbf{r}}{V}}$

Scattering by many impurities



Impurity locations are R_1, R_2, … They are "uncorrelated"

$$W_{total}(\mathbf{r}) = \underbrace{W(\mathbf{r}) + W(\mathbf{r}-\mathbf{R_1}) + W(\mathbf{r}-\mathbf{R_2}) + \ldots}_{`N'_{imp}impurities}$$

$$V_0(\mathbf{q}) \approx \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r})\frac{d^3\mathbf{r}}{V}$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + \int_V e^{i\mathbf{q}\cdot\mathbf{r}}W(\mathbf{r}-\mathbf{R_1})\frac{d^3\mathbf{r}}{V} + \ldots$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q}) + V_0(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R_1}} + V_0(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots$$

$$V_{total}(\mathbf{q}) = V_0(\mathbf{q})[\underbrace{1 + e^{i\mathbf{q}\cdot\mathbf{R_1}} + e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{`N'terms}]$$

$$|V_{total}(\mathbf{q})|^2 = |V_0(\mathbf{q})|^2[(\underbrace{1 + e^{i\mathbf{q}\cdot\mathbf{R_1}} + e^{i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{`N'_{imp}terms})\times(\underbrace{1 + e^{-i\mathbf{q}\cdot\mathbf{R_1}} + e^{-i\mathbf{q}\cdot\mathbf{R_2}}\ldots}_{`N'_{imp}terms})]$$

$$|V_{total}(\mathbf{q})|^2 = |V_0(\mathbf{q})|^2[N_{imp} + (\underbrace{e^{i\mathbf{q}\cdot(\mathbf{R_1}-\mathbf{R_2})} + e^{i\mathbf{q}\cdot(\mathbf{R_1}-\mathbf{R_3})}\ldots}_{\approx 0(RPA)})]$$

Fourier Transform property:

$$\int e^{iqx}f(x)dx \leftrightarrow F(q)$$

$$\int e^{iqx}f(x+a)dx \leftrightarrow F(q)\times e^{iqa}$$

Effect of multiple scattering

$$|V_{total}(\mathbf{q})|^2 = N_{imp}|V_0(\mathbf{q})|^2$$

$$\boxed{\frac{1}{\tau_{\mathbf{kk'}}(total)} = \frac{2\pi}{\hbar}N_{imp}\times|V_0(\mathbf{q})|^2\delta[E_{\mathbf{k'}} - (E_{\mathbf{k}} \pm \hbar\omega)]}$$

Scattering rate is <u>linearly proportional to impurity density</u> in the dilute uncorrelated limit!

(c) Ionized Impurity Scattering

Screened Coulomb potential

$$W(r) = -\frac{Ze^2}{4\pi\epsilon_s r}e^{-\frac{r}{L_D}} \tag{1}$$

Scattering rate is given by Fermi Golden rule as :

$$S(k \to k') = \frac{2\pi}{\hbar} * |<\vec{k'}|W(r)|\vec{k}>|^2 * \delta(E_k - E_{k'})$$

Matrix element :

$$<\vec{k'}|W(r)|\vec{k}> \approx \int d^3r \left(\frac{e^{-i\vec{k'}\cdot\vec{r}}}{\sqrt{V}}\right)\left(-\frac{Ze^2}{4\pi\epsilon_s r}e^{-\frac{r}{L_D}}\right)\left(\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\right)$$

Assuming the scattering is in the same band, the Bloch parts integrate out to 1 and only the envelope parts remain.

$$= \int r^2 \sin\theta \, dr \, d\theta \, d\phi \, \frac{e^{i\vec{Q}\cdot\vec{r}}}{V}\left(-\frac{Ze^2}{4\pi\epsilon_s r}e^{-\frac{r}{L_D}}\right)$$

where $\vec{Q} = \vec{k'} - \vec{k}$

$$\begin{aligned}
&= -\frac{Ze^2}{4\pi\epsilon_s r V}\int_{\phi=0}^{2\pi} d\phi \int_{r=0}^{\infty} dr \, r e^{-r/L_D} \int_{\theta=0}^{\pi} d\theta \sin\theta e^{iQr\cos\theta} \\
&= -\frac{Ze^2}{\epsilon_s Q V}\underbrace{\int_{r=0}^{\infty} dr \sin(Qr) e^{-r/L_D}}_{\frac{Q}{\frac{1}{L_D^2}+Q^2}} \\
<\vec{k'}|W(r)|\vec{k}> &= -\frac{Ze^2}{\epsilon_s V\left(\frac{1}{L_D^2}+Q^2\right)}
\end{aligned}$$

Therefore scattering rate of state k to k':

$$S(k \to k') = \frac{2\pi}{\hbar} * \left(-\frac{Ze^2}{\epsilon_s V\left(\frac{1}{L_D^2}+Q^2\right)}\right)^2 * \delta(E_k - E_{k'})$$

Total scattering rate of state k :

$$\frac{1}{\tau(k)} = \sum_{k'} S(k \to k')(1 - \cos\theta)$$

Here $\tau = \tau_m$, the momentum scattering time and θ is the angle between $\vec{k}$ and $\vec{k'}$

$$\begin{aligned}
\frac{1}{\tau(k)} &= \sum_{k'} S(k \to k')(1-\cos\theta) \\
&= \sum_{k'} \frac{2\pi}{\hbar} * \left(-\frac{Ze^2}{\epsilon_s V\left(\frac{1}{L_D^2}+Q^2\right)}\right)^2 * \delta(E_k - E_{k'})(1-\cos\theta)
\end{aligned}$$

Now,

$$\begin{aligned}
Q^2 = |\vec{k} - \vec{k'}|^2 &= |k|^2 + |k'|^2 - 2|k||k'|\cos\theta \\
&= \underbrace{2k^2(1-\cos\theta)}_{Elastic\ scattering} \\
\implies 1 - \cos\theta &= \frac{Q^2}{2k^2}
\end{aligned}$$

And,

$$\begin{aligned}
E_k - E_{k'} &= \frac{\hbar^2}{2m_c^*}|k|^2 - \frac{\hbar^2}{2m_c^*}|k'|^2 \\
&= \frac{\hbar^2}{2m_c^*}(k^2 - k'^2) \\
\implies \delta(E_k - E_{k'}) &= \frac{2m_c^*}{\hbar^2} * \delta(k^2 - k'^2) \\
&= \frac{2m_c^*}{\hbar^2} * \delta\left[\underbrace{(k+k')}_{=2k}(k-k')\right] \\
&= \frac{m_c^*}{\hbar^2 k} * \delta(k - k')
\end{aligned}$$

Substituting, we get :

$$\begin{aligned}
\frac{1}{\tau(k)} &= \sum_{k'} \frac{2\pi}{\hbar} * \left(-\frac{Ze^2}{\epsilon_s V\left(\frac{1}{L_D^2}+Q^2\right)}\right)^2 * \delta(E_k - E_{k'})(1-\cos\theta) \\
&= \sum_{k'} \frac{2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2 V^2\left(\frac{1}{L_D^2}+Q^2\right)^2}\frac{Q^2}{2k^2}\frac{m_c^*}{\hbar^2 k} * \delta(k-k') \\
&= \frac{2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V^2}\frac{m_c^*}{2\hbar^2}\cdot\sum_{k'}\frac{|k-k'|^2}{\left(\frac{1}{L_D^2}+|k-k'|^2\right)^2}\cdot\frac{1}{k^3}\cdot\delta(k-k') \\
&= \frac{g_sg_v2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V^2}\frac{m_c^*}{2\hbar^2}\cdot\int_{k'}\frac{d^3k'}{(2\pi)^3/V}\frac{|k-k'|^2}{\left(\frac{1}{L_D^2}+|k-k'|^2\right)^2}\cdot\frac{1}{k^3}\cdot\delta(k-k') \\
&= \frac{g_sg_v2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V(2\pi)^3}\frac{m_c^*}{2\hbar^2}\cdot\int_{k'}k'^2\sin\theta\,dk'\,d\theta\,d\phi\,\frac{|k-k'|^2}{\left(\frac{1}{L_D^2}+|k-k'|^2\right)^2}\cdot\frac{1}{k^3}\cdot\delta(k-k') \\
&= \frac{g_sg_v2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V(2\pi)^3}\frac{m_c^*}{2\hbar^2}\cdot\int_{\phi=0}^{2\pi}d\phi\int_{\theta=0}^{\pi}d\theta\sin\theta\int_{k'=0}^{\infty}k'^2\,dk'\,\frac{2k^2(1-\cos\theta)}{\left(\frac{1}{L_D^2}+|k-k'|^2\right)^2}\cdot\frac{1}{k^3}\cdot\delta(k-k') \\
&= \frac{g_sg_v2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V(2\pi)^3}\frac{m_c^*}{2\hbar^2}\cdot 2\pi\cdot 2k\int_{\theta=0}^{\pi}d\theta\sin\theta\frac{(1-\cos\theta)}{\left(\frac{1}{L_D^2}+2k^2(1-\cos\theta)\right)^2} \\
&= \frac{g_sg_v2\pi}{\hbar}\frac{Z^2e^4}{\epsilon_s^2V(2\pi)^3}\frac{m_c^*}{2\hbar^2}\cdot 2\pi\cdot 2k\left[\frac{1}{4k^4}\left(ln(1+4k^2L_D^2) - \frac{4k^2L_D^2}{1+4k^2L_D^2}\right)\right] \\
\implies \frac{1}{\tau(k)} &= \frac{g_sg_vZ^2e^4m_c^*}{8\pi\hbar^3\epsilon_s^2V}\cdot\frac{1}{k^3}\left(ln(1+4k^2L_D^2) - \frac{4k^2L_D^2}{1+4k^2L_D^2}\right)
\end{aligned}$$

Check dimensions!

Kinetic energy :

$$\begin{aligned}
E(k) &= \frac{\hbar^2k^2}{2m_c^*} \\
\implies k^3 &= \left(\frac{2m_c^*E}{\hbar^2}\right)^{3/2}
\end{aligned}$$

Substituting, scattering due to **single impurity**,

$$\frac{1}{\tau(E)} = \frac{g_sg_vZ^2e^4m_c^*}{8\pi\hbar^3\epsilon_s^2V}\cdot\frac{1}{\left(\frac{2m_c^*E}{\hbar^2}\right)^{3/2}}\left(ln(1+\frac{8m_c^*E}{\hbar^2}L_D^2) - \frac{\frac{8m_c^*E}{\hbar^2}L_D^2}{1+\frac{8m_c^*E}{\hbar^2}L_D^2}\right)$$

scattering due to**N uncorrelated impurities in volume V**,

$$\begin{aligned}
\frac{1}{\tau^{tot}(E)} &= \frac{N}{\tau(E)} \\
&= \frac{g_sg_vZ^2e^4m_c^*}{8\pi\hbar^3\epsilon_s^2}\cdot\underbrace{\frac{N}{V}}_{=N_D}\cdot\frac{1}{\left(\frac{2m_c^*E}{\hbar^2}\right)^{3/2}}\left(ln(1+\frac{8m_c^*E}{\hbar^2}L_D^2) - \frac{\frac{8m_c^*E}{\hbar^2}L_D^2}{1+\frac{8m_c^*E}{\hbar^2}L_D^2}\right) \\
\implies \tau^{tot}(E) &= \frac{8\pi\hbar^3\epsilon_s^2}{g_sg_vZ^2e^4m_c^*N_D}\left(\frac{2m_c^*E}{\hbar^2}\right)^{3/2}\cdot\left(ln(1+\frac{8m_c^*E}{\hbar^2}L_D^2) - \frac{\frac{8m_c^*E}{\hbar^2}L_D^2}{1+\frac{8m_c^*E}{\hbar^2}L_D^2}\right)^{-1}
\end{aligned}$$

Now, mobility μ :

$$\begin{aligned}
\mu &= \frac{e<\tau>}{m_c^*} \\
<\tau> &= \frac{2}{d}\cdot\frac{\int dE\tau(E)E^{d/2}\frac{-\partial f_o}{\partial E}}{\int dEE^{d/2-1}\partial f_o(E)}
\end{aligned}$$

Here $f_o \approx e^{-E/kT}$ and $\frac{-\partial f_o}{\partial E} = \frac{1}{kT}e^{-E/kT}$, and dimension $d = 3$

$$<\tau> = \frac{2}{3}\cdot\frac{\int dE\tau^{tot}(E)E^{3/2}\frac{1}{kT}e^{-E/kT}}{\int dEE^{1/2}e^{-E/kT}}$$

Let $E = u.kT$

$$\begin{aligned}
<\tau> &= \frac{2}{3}\cdot\frac{\int_0^\infty du\,\tau^{tot}(u)u^{3/2}e^{-u}}{\underbrace{\int_0^\infty du\,u^{1/2}e^{u}}_{\Gamma(1/2)=\sqrt{\pi}}} \\
&= \frac{2}{3\sqrt{\pi}}\cdot\int_0^\infty du\,u^{3/2}e^{-u}\cdot\tau^{tot}(u)
\end{aligned}$$

$$\tau^{tot}(u) = \frac{8\pi\hbar^3\epsilon_s^2}{g_sg_vZ^2e^4m_c^*N_D}\left(\frac{2m_c^*kT}{\hbar^2}\right)^{3/2}.u^{3/2}\cdot\left(ln(1+u.\frac{8m_c^*}{\hbar^2}L_D^2) - \frac{u.\frac{8m_c^*}{\hbar^2}L_D^2}{1+u.\frac{8m_c^*}{\hbar^2}L_D^2}\right)^{-1}$$

$$
\begin{aligned}
<\tau> &= \frac{2}{3\sqrt{\pi}} \cdot \int_0^\infty du\, u^{3/2} e^{-u} \cdot \tau^{tot}(u) \\
&= \frac{2}{3\sqrt{\pi}} \cdot \int_0^\infty du\, u^{3/2} e^{-u} \cdot \frac{8\pi\hbar^3\epsilon_s^2}{g_s g_v Z^2 e^4 m_c^* N_D} \left(\frac{2m_c^* kT}{\hbar^2}\right)^{3/2} .u^{3/2} \\
&\cdot \underbrace{\left(ln(1 + u.\frac{8m_c^*}{\hbar^2} L_D^2) - \frac{u.\frac{8m_c^*}{\hbar^2} L_D^2}{1 + u.\underbrace{\frac{8m_c^*}{\hbar^2} L_D^2}_{x}} \right)^{-1}}_{\text{slowly varying in x}} \\
&= \frac{2}{3\sqrt{\pi}} \frac{8\pi\hbar^3\epsilon_s^2}{g_s g_v Z^2 e^4 m_c^* N_D} \left(\frac{2m_c^* kT}{\hbar^2}\right)^{3/2} \int_0^\infty du\, e^{-u} \underbrace{\frac{\overbrace{u^3}^{\text{Fast varying}}}{ln(1+ux) - \frac{ux}{1+ux}}}_{\text{Slow varying}} \\
&\approx \frac{2}{3\sqrt{\pi}} \frac{8\pi\hbar^3\epsilon_s^2}{g_s g_v Z^2 e^4 m_c^* N_D} \left(\frac{2m_c^* kT}{\hbar^2}\right)^{3/2} \cdot \frac{1}{\underbrace{D(u)}_{\text{Use D(u=3)}}} \overbrace{\int_0^\infty du\, \underbrace{e^{-u} u^3}_{\text{Max at u=3}}}^{\Gamma(3)=2} \\
&\approx \frac{4}{3\sqrt{\pi}} \frac{8\pi\hbar^3\epsilon_s^2}{g_s g_v Z^2 e^4 m_c^* N_D} \left(\frac{2m_c^* kT}{\hbar^2}\right)^{3/2} \cdot \frac{1}{ln(1+\beta^2) - \frac{\beta^2}{1+\beta^2}}
\end{aligned}
$$

Where $\beta = 2\sqrt{\frac{2m_c^* 3kT}{\hbar^2}}.L_D$

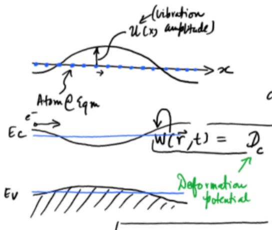
Therefore, mobility

$$
\begin{aligned}
\mu &= \frac{e <\tau>}{m_c^*} \\
&\approx \frac{e}{m_c^*} \cdot \frac{4}{3\sqrt{\pi}} \frac{8\pi\hbar^3\epsilon_s^2}{g_s g_v Z^2 e^4 m_c^* N_D} \left(\frac{2m_c^* kT}{\hbar^2}\right)^{3/2} \cdot \underbrace{\frac{1}{ln(1+\beta^2) - \frac{\beta^2}{1+\beta^2}}}_{F(\beta)} \\
\mu &\approx \left[\frac{2^{7/2}}{6\pi^{3/2}} \frac{(4\pi\epsilon_s)^2}{Z^2 e^3 g_s g_v \sqrt{m_c^*} F(\beta)} \right] \frac{(kT)^{3/2}}{N_D} \propto \frac{T^{3/2}}{N_D}
\end{aligned}
$$

That was a long calculation!

(d) Acoustic Phonon Scattering

$\boxed{\text{Problem 27}}$ $\boxed{\text{Phonon Scattering}}$



If the displacement of the atom @ $\vec{r}$ is $\vec{u}(\vec{r})$, the perturbation potential due to an acoustic phonon is

$$\boxed{W(\vec{r},t) = \underbrace{D_c}_{\text{Deformation potential}} \underbrace{\nabla_r \cdot \vec{u}(\vec{r},t)}_{\text{Local strain}}}$$

$$\boxed{\vec{u}(\vec{r},t) = \underbrace{\hat{n}}_{\text{direction of vibration}} \underbrace{u_0}_{\text{amplitude of vibration}} e^{i(\vec{q}\cdot\vec{r} - \omega t)}}$$

$\frac{2\pi}{\lambda}\hat{q}$, $\omega = v_s q$ (Sound velocity for LA mode)

LA: $\hat{n} \parallel \hat{q}$

TA: $\hat{n} \perp \hat{q}$

$2M\omega_q^2 u_0^2 \approx N_{ph} \cdot \hbar\omega_q$

$$\Rightarrow \boxed{u_0 \approx \sqrt{\frac{\hbar}{2\rho\Omega\omega_q}} \cdot \sqrt{N_{ph}}}$$

The $e^{i\omega t}$ terms go to conserve energy: $\delta(E_k - E_{k'} \pm \hbar\omega)$

$$\frac{1}{\tau(\vec{k}\to\vec{k}')} = S(\vec{k}\to\vec{k}') = \frac{2\pi}{\hbar} \underbrace{|\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle|^2}_{\text{Matrix element, need } W(\vec{r}) \text{ to evaluate}} \delta(\mathcal{E}_k - \mathcal{E}_{k'} \pm \hbar\omega)$$

$$W(\vec{r},t) = D_c \cdot \nabla_r \cdot \hat{n} u_0 e^{i(\vec{q}\cdot\vec{r} - \omega t)}$$

$$= i D_c u_0 (\hat{n}\cdot\vec{q}) e^{i(\vec{q}\cdot\vec{r} - \omega t)}$$

$$= \underbrace{\left[i D_c u_0 (\hat{n}\cdot\vec{q}) e^{i\vec{q}\cdot\vec{r}}\right]}_{W(\vec{r})} \underbrace{\left[e^{-i\omega t}\right]}_{\text{Energy Conservation}}$$

$W(\vec{r}) = 0$ for TA modes because $\hat{n} \perp \vec{q}$

$\neq 0$ for LA modes because $\hat{n} \parallel \vec{q}$

$\therefore$ For LA modes:

$$W(\vec{r}) = i D_c u_0 q e^{i\vec{q}\cdot\vec{r}}$$

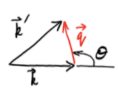
Matrix element:

$$\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle = \int d^3r \cdot \left(\frac{e^{-i\vec{k}'\cdot\vec{r}}}{\sqrt{V}}\right) \cdot \left(i D_c u_0 q e^{i\vec{q}\cdot\vec{r}}\right) \cdot \left(\frac{e^{+i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\right)$$

(Envelope function assuming scattering within the same band, Bloch-periodic parts integrate to 1)

$$\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle = \int \frac{d^3r}{V} e^{i(\vec{k}-\vec{k}'+\vec{q})\cdot\vec{r}} \cdot i D_c u_0 q$$

$$= i D_c u_0 q \cdot \underbrace{\int \frac{d^3r}{V} e^{i(\vec{k}-\vec{k}'+\vec{q})\cdot\vec{r}}}_{}$$



$= \delta_{\vec{k}', \vec{k}+\vec{q}}$ ← Kronecker Delta, $\begin{cases} =1 & \text{for } \vec{k}' = \vec{k}+\vec{q} \\ =0 & \text{for } \vec{k}' \neq \vec{k}+\vec{q} \end{cases}$

"Momentum Conservation"

$$\therefore \boxed{\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle = i D_c u_0 q \, \delta_{\vec{k}', \vec{k}+\vec{q}}}$$

$$\begin{cases} \vec{k}' = \vec{k} \pm \vec{q} \\ k'^2 = k^2 + q^2 \pm 2kq\cos\theta \end{cases}$$

$$S(\vec{k}\to\vec{k}') = \frac{2\pi}{\hbar} |\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle|^2 \delta(E_k - E_{k'} + \hbar\omega)$$

$$|\langle \vec{k}'|W(\vec{r})|\vec{k}\rangle|^2 = D_c^2 u_0^2 q^2 \cdot \delta_{\vec{k}', \vec{k}+\vec{q}} \qquad \left\{ \text{Note: } \delta_{a,b}^2 = \delta_{a,b} \right\}$$

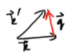
$$\Rightarrow S(\vec{k}\to\vec{k}') = \frac{2\pi}{\hbar} D_c^2 u_0^2 q^2 \cdot \underbrace{\delta_{\vec{k}', \vec{k}\pm\vec{q}}}_{\substack{\text{Kronecker-Delta} \\ \text{Momentum Conservation}}} \cdot \underbrace{\delta(E_k - E_{k'} \pm \hbar\omega)}_{\substack{\text{Dirac-Delta} \\ \text{Energy Conservation}}}$$

Energy conservation:

$$\frac{\hbar^2 k'^2}{2m_c^*} = \frac{\hbar^2 k^2}{2m_c^*} \pm \hbar\omega_q \leftarrow \omega_q \approx v_s \cdot q \leftarrow (\text{Low-energy Acoustic phonons})$$

(sound velocity: v_s)

$$\underbrace{\boxed{k'^2 = k^2 \pm \frac{2m_c^* v_s \cdot q}{\hbar}}}_{\text{Energy Conservation}} \leftrightarrow \underbrace{\boxed{k'^2 = k^2 + q^2 \pm 2kq\cos\theta}}_{\text{Momentum Conservation}}$$



$$\pm \frac{2m_c^*}{\hbar} v_s q = q^2 \pm 2kq\cos\theta$$

$$\begin{pmatrix} q_{min} \approx 0 \\ q_{max} \approx 2k \end{pmatrix} \begin{pmatrix} \text{quasi-} \\ \text{elastic} \end{pmatrix} \Leftarrow \boxed{q = \pm \frac{2m_c^* v_s}{\hbar} \mp 2k\cos\theta} \quad \text{Relation between } [k, q, + \theta]$$

$$S(\vec{k}\to\vec{k}') = S(\vec{k},\vec{q}) = \frac{2\pi}{\hbar} D_c^2 u_0^2 q^2 \, \delta\left[\frac{\hbar^2 k^2}{2m_c^*} - \frac{\hbar^2}{2m_c^*}(k^2+q^2 \pm 2kq\cos\theta) \pm \hbar v_s q\right]$$

$$= \frac{2\pi}{\hbar} D_c^2 u_0^2 q^2 \, \delta\left[-\frac{\hbar^2 q^2}{2m_c^*} \mp \frac{\hbar^2 kq}{m_c^*}\cos\theta \pm \hbar v_s q\right]$$

$$= \frac{2\pi}{\hbar} D_c^2 u_0^2 q^2 \, \delta\left[\underbrace{-\frac{\hbar^2 kq}{m_c^*}}\left(\pm\cos\theta + \frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}\right)\right]$$

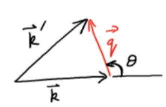
$$\delta(ax) = \frac{1}{|a|}\delta(x)$$

$$= \frac{2\pi}{\hbar} D_c^2 u_0^2 q^2 \cdot \frac{m_c^*}{\hbar^2 kq} \, \delta\left[\pm\cos\theta + \frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}\right]$$

$$\boxed{S(\vec{k},\vec{q}) = \frac{2\pi D_c^2 u_0^2 m_c^* q}{\hbar^3 k} \, \delta\left[\pm\cos\theta + \frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}\right]}$$

Units $= \frac{1}{s}$

$$\frac{1}{\tau_m(k)} = \sum_q S(\vec{k},\vec{q}) \cdot \left(1 - \frac{\vec{k}\cdot\vec{k}'}{k^2}\right)$$



$$\vec{k}' = \vec{k} \pm \vec{q}$$

$$1 - \frac{\vec{k}\cdot\vec{k}'}{k^2} = 1 - \frac{\vec{k}\cdot(\vec{k}\pm\vec{q})}{k^2}$$

$$= \mp \frac{\vec{k}\cdot\vec{q}}{k^2} = \mp \frac{q\cos\theta}{k}$$

$$u_0^2 = \frac{\hbar}{2\rho\Omega\omega_q} \cdot N_{ph}$$

$$\approx \frac{\hbar}{2\rho\Omega v_s q} \cdot \frac{k_B T}{\hbar\omega_q}$$

$$\boxed{u_0^2 \approx \frac{k_B T}{2\rho\Omega v_s^2 q^2}}$$

$$\Rightarrow \frac{1}{\tau_m(k)} = \sum_q S(\vec{k},\vec{q}) \cdot \left(\mp \frac{q\cos\theta}{k}\right)$$

$$= \sum_q \frac{2\pi D_c^2 u_0^2 m_c^* q}{\hbar^3 k} \left(\mp \frac{q\cos\theta}{k}\right) \cdot \delta\left[\pm\cos\theta + \frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}\right]$$

$$= \int \frac{q^2 \sin\theta \, dq \, d\theta \, d\phi}{\frac{(2\pi)^3}{V}} \cdot \mp \frac{2\pi D_c^2 u_0^2 m_c^* q^2 \cos\theta}{\hbar^3 k^2} \cdot \delta\left[\pm\cos\theta + \frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}\right]$$

$$= \mp \frac{k_b T}{2\rho\Omega v_s^2} \frac{2\pi D_c^2 m_c^*}{\frac{(2\pi)^3}{V} \cdot \hbar^3 \cdot k^2} \cdot \int_{\phi=0}^{2\pi} d\phi \cdot \int_{q=q_{min}}^{q_{max}} dq \cdot \frac{q^4}{q^2} \cdot \underbrace{\int_{\theta=0}^{\pi} d\theta \cdot \sin\theta \cdot \cos\theta \cdot \delta\Big[\pm\cos\theta + \underbrace{\frac{q}{2k} \mp \frac{m_c^* v_s}{\hbar k}}_{u_0}\Big]}$$

$$\cos\theta = u \qquad d\theta \sin\theta = -du$$

$$\boxed{\int (-du) \cdot u \cdot \delta\Big[\pm u - \big(\underbrace{\pm \frac{m_c^* v_s}{\hbar k}}_{u_0} - \frac{q}{2k}\big)\Big] = \pm u_0 = \pm \frac{m_c^* v_s}{\hbar k} \mp \frac{q}{2k}}$$

$$\frac{1}{\tau_m(k)} = \mp \frac{k_b T}{2\rho\Omega v_s^2} \frac{\cancel{2\pi} D_c^2 m_c^*}{2\pi \frac{\cancel{(2\pi)^3}}{V} \cdot \hbar^3 k^2} \cdot \cancel{2\pi} \cdot \int_{q=0}^{q=2k} dq \cdot q^2 \left(\pm \frac{m_c^* v_s}{\hbar k} \mp \frac{q}{2k}\right)$$

$$= \mp \frac{V \cdot D_c^2 m_c^* \cdot k_b T}{4\pi\rho\Omega v_s^2 \hbar^3 k^2} \cdot \left[\pm \frac{m_c^* v_s}{\hbar} \frac{8k^3}{3k} \mp \frac{16k^4}{4 \cdot 2k}\right]$$

$$= \mp \frac{V \cdot D_c^2 m_c^* k_b T}{4\pi\rho\Omega v_s^2 \hbar^3} \left(\pm \frac{8 m_c^* v_s}{3\hbar} \mp 2k\right)$$

$$= \frac{V \cdot D_c^2 m_c^* k_b T}{2\pi\rho\Omega v_s^2 \hbar^3} \cdot k \cdot \left(1 \pm \frac{v_s}{\frac{3}{8}\frac{\hbar k}{m_c^*}}\right)$$

Sound velocity

electron group velocity

$\ll 1$

$\Rightarrow$ neglect!

$$\frac{1}{\tau_m(k)} \simeq \frac{V \cdot D_c^2 m_c^* k_b T}{2\pi\rho\Omega v_s^2 \hbar^3} \cdot k$$

$$\frac{\hbar^2 k^2}{2m_c^*} = \varepsilon \qquad k = \sqrt{\frac{2m_c^*}{\hbar^2}} \cdot \sqrt{\varepsilon}$$

$$\tau_m(\varepsilon) \simeq \frac{2\pi\rho\Omega v_s^2 \hbar^3}{V \cdot D_c^2 m_c^* k_b T} \cdot \frac{1}{\sqrt{\frac{2m_c^*}{\hbar^2}}} \cdot \frac{1}{\sqrt{\varepsilon}}$$

$$\simeq \frac{\sqrt{2}\pi\rho\Omega v_s^2 \hbar^4}{V \cdot D_c^2 (m_c^*)^{3/2} k_b T} \cdot \varepsilon^{-1/2}$$

$C_L =$

$$\rho v_s^2 = \frac{kg}{m^3} \frac{m^2}{s^2} = \frac{kg}{m^2} \cdot \frac{m}{s^2} = \frac{Force}{m^2}$$

$$\Downarrow$$

$$\mu = \frac{e\langle\tau_m\rangle}{m_c^*} \propto \frac{e\hbar^4 \rho v_s^2}{D_c^2 (m_c^*)^{5/2} (k_b T)^{3/2}} \propto T^{-3/2}$$

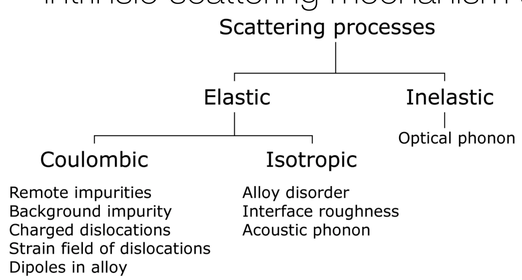
Another longish (but mostly mechanical calculation of acoustic phonon scattering rates in semiconductors).

(e) Optical Phonon scattering: I have included some figures from the slides used in class. The major difference between optical phonons and acoustic phonon modes:
- in acoustic phonon modes, neighboring atoms vibrate in phase, whereas
- in optical phonon modes, neighboring atoms vibrate out of phase.

Optical phonon scattering can occur by
- a non-polar deformation potential coupling due to strain of the crystal and resulting perturbation of the band edge energies. Unlike the acoustic phonon, the optical deformation potential has units of Dop~eV/Angstrom and unlike the strain field, it is the direct displacement of the atoms that

enters the perturbation matrix element, i.e. W(r) ~ Dop*d(x1-x2) where d(x1-x2) is the relative displacement of the nearest neighbor atoms in the crystal. This form of "mechanical" or strain-induced non-polar (non-Coulombic) scattering occurs in elemental semiconductors such as Si and Ge, which lack polar optical phonon modes and serves as the important means of energy loss of high-energy or hot electrons.

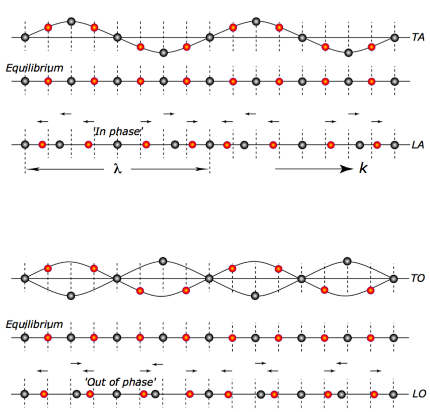
- Polar-optical phonon scattering occurs in polar crystals such as GaAs, GaN, etc that have two atoms of different ionicities in the basis of the crystal. This form of scattering is due to the vibration of effectively charged ions causing a dipole field, and the scattering is of Coulombic nature, and is therefore typically much stronger and dominates non-polar kinds. Polar optical phonon scattering is typically the strongest scattering mechanism at room temperature for GaAs, GaN, and all III-V semiconductors. In other words, it limits the mobility and the performance of several high-speed transistors, light-emitting diodes and lasers, etc as it is the dominant low-field scattering mechanism at room temparuture that cannot be decreased by making the materials purer – because it is an intrinsic scattering mechanism and not tied to defects.

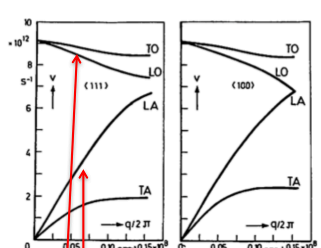


A static periodic potential causes no scattering → every other potential causes scattering!

Periodic 'non-static' potentials: ***Phonons****.*
Static non-periodic potentials: ***Defects*** *&* ***Impurities****.*

Classification of scattering mechanisms





Acoustic and optical phonon dispersion

$$\omega_{\pm}^2(k) = \frac{C}{M_r}[1 \pm \sqrt{1 - \frac{2M_r}{M_1 + M_2}(1 - \cos ka)}]$$

Optical vs Acoustic modes

Electron-Phonon Scattering Rates

Polar optical phonon

$$D = \epsilon_0 E + \frac{q^\star u}{\Omega}$$

$$E(x,t) = -\frac{q q^\star u}{\epsilon_0 \Omega}$$

$$W(r,t) = -q\int dx E(x,t) = \frac{q}{i\beta\epsilon_0}\cdot\frac{q^\star}{\Omega}\cdot u_0 e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$$

$$\left(\frac{q^\star}{\Omega}\right)^2 = \rho\epsilon_0\omega_0^2\left(\frac{1}{\epsilon_s^\infty}-\frac{1}{\epsilon_s^0}\right)$$

$$W(r,t) = -q\int dx E(x,t) = \frac{q\omega_0\sqrt{\rho}}{i\beta}\sqrt{\frac{1}{\epsilon_s^\infty}-\frac{1}{\epsilon_s^0}}\cdot u_0 e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$$

Piezoelectric acoustic phonon

$$D = \epsilon_0\epsilon_s E + e_{pz}\frac{\partial u}{\partial x}$$

$$E(x,t) = -\frac{e_{pz}}{\epsilon_0\epsilon_s}\frac{\partial u}{\partial x}$$

$$W(r,t) = -q\int dx E(x,t) = \frac{q e_{pz}}{\epsilon_0\epsilon_s} u_0 e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$$

$$\frac{K^2}{1-K^2} = \frac{e_{pz}^2}{\epsilon_0\epsilon_s v_s}$$

$$S(k\to k') = \frac{2\pi}{\hbar}|W(q_s)|^2\frac{\hbar}{2\rho\Omega\omega_{q_s}}[N(\omega_{q_s})+\frac{1}{2}\mp\frac{1}{2}]\delta[\pm\cos(\theta)+\frac{q_s}{2k}\mp\frac{\omega_{q_s}}{v q_s}]$$

Deformation potential acoustic phonon

$$W(x,t) = D_{ac}\frac{\partial u}{\partial x}$$

$$W(r,t) = D_{ac}(\nabla\cdot\mathbf{u}) = iD_{ac}\beta u_0 e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$$

Deformation potential optical phonon

$$W(r,t) = D_{op}u = D_{op}u_0 e^{i(\boldsymbol{\beta}\cdot\mathbf{r}-\omega t)}$$

Momentum conservation

$$\hbar\mathbf{k}' = \hbar\mathbf{k}\pm\hbar\boldsymbol{\beta}$$

Energy conservation

$$E_{\mathbf{k}'} = E_{\mathbf{k}}\pm\hbar\omega_{\boldsymbol{\beta}}$$

$$k'^2 = k^2+\beta^2\pm 2k\beta\cos\theta$$

Energy conservation

$$\beta^2\pm 2\beta k\cos\theta\mp\frac{2m^\star\hbar\omega_\beta}{\hbar^2} = 0$$

For acoustic phonons, $\hbar\omega_\beta = \hbar v_s\beta$, and we get

Allowed angles for acoustic phonon scattering events

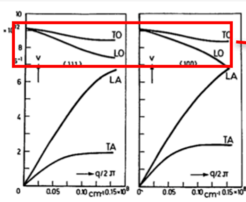
$$\beta = 2k(\mp\cos\theta\pm\frac{m^\star v_s}{\hbar k}) = 2k(\mp\cos\theta\pm\frac{v_s}{v_k})$$

For optical phonons, we get

Allowed angles for optical phonon scattering events

$$\beta = \mp k\cos\theta\pm\sqrt{k^2\cos^2\theta\pm\frac{2m^\star\hbar\omega_\beta}{\hbar^2}}$$

Electron-Optical Phonon Scattering Rates, Mobility



$\hbar\,\omega_0 = k_B\Theta$.

Θ is known as the *Debye temperature*

Deformation potential Optical Phonon

$$\mu_0 = \frac{4\sqrt{2\pi}\,e\,\hbar^2\varrho(k_B\Theta)^{1/2}}{3m^{5/2}D^2}f(T/\Theta)\,.$$

The function $f(T/\Theta)$ is given by

$$f(T/\Theta) = (2z)^{5/2}(e^{2z}-1)\int_0^\infty\frac{y^{3/2}e^{-2zy}\,dy}{\sqrt{y+1}+e^{2z}\,\mathrm{Re}\{\sqrt{y-1}\}},$$

where $z = \Theta/2T$ and $y = \varepsilon/k_B\Theta$. The function is shown

Its numerical value in units of cm²/V s is given by

$$\mu = 2.04\times10^3\frac{(\varrho/\mathrm{g\,cm^{-3}})(\Theta/400\,\mathrm{K})^{1/2}}{(m/m_0)^{5/2}(D/10^8\,\mathrm{eV\,cm^{-1}})^2}f(T/\Theta)$$

Polar Optical Phonon Scattering

$$\alpha = \frac{\hbar\,|e|\,E_0}{2^{1/2}m^{1/2}(\hbar\,\omega_0)^{3/2}} = \frac{1}{137}\sqrt{\frac{m\,c^2}{2k_B\Theta}}\left(\frac{1}{\varkappa_{opt}}-\frac{1}{\varkappa}\right)$$

$$= 397.4\sqrt{\frac{m/m_0}{\Theta/\mathrm{K}}}\left(\frac{1}{\varkappa_{opt}}-\frac{1}{\varkappa}\right)$$

The mobility is simply $(e/m)\,\tau_m$:

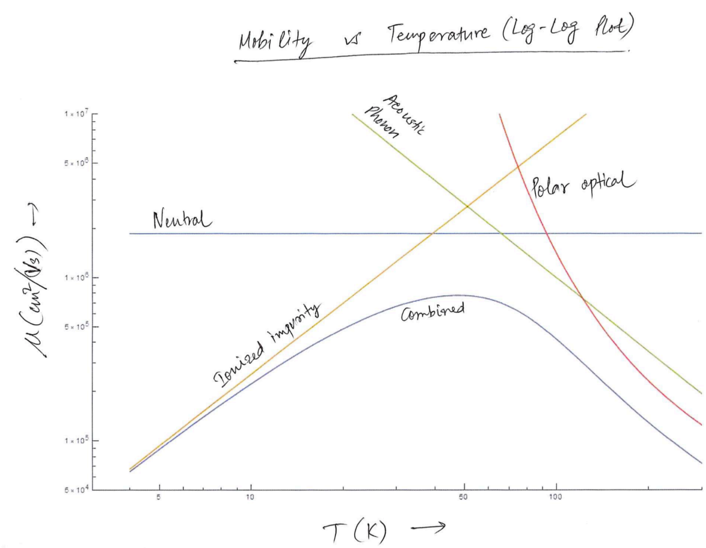
$$\mu = [|e|/(2m\,\alpha\,\omega_0)]\exp(\Theta/T)$$

which in units of cm²/V s is given by

$$\mu = 2.6\times10^5\frac{\exp(\Theta/T)}{\alpha(m/m_0)(\Theta/\mathrm{K})}\quad\text{for}\quad T\ll\Theta$$

For example, in n-type GaAs where $\Theta = 417$ K, $m/m_0 = 0.072$, $\alpha = 0.067$, we calculate a mobility at 100 K of 2.2×10^5 cm²/V s. This is of the order of magnitude of the highest mobilities observed in this material. At this and

Expressions for optical phonon scattering rates (f): Example Plot from Sayak Ghosh's 2017 solution. The numbers are a bit on the high side (for example the 300K mobility of GaAs is less than 10000 cm^2/Vs, this calculation overestimates the optical phonon mobility number by ~10 X, but all other trends are reasonable. The neutral impurity concentration should be calculated as a function of temperature using charge-neutrality conditions, meaning as dopants are thermally activated at high temperatures, the neutral impurity density decreases, and the mobility due to neutral impurity scattering alone should increase as shown in the original paper.



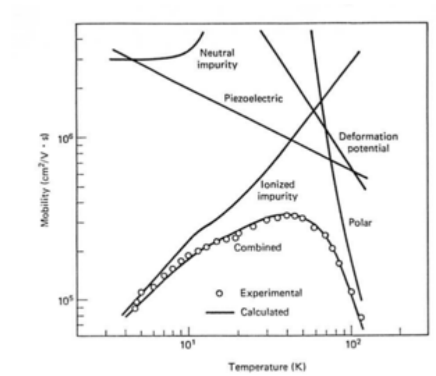


Figure 6.7 Temperature dependence of the mobility for *n*-type GaAs showing the separate and combined scattering processes. [From C. M. Wolfe, G. E. Stillman, and W. T. Lindley, *J. Appl. Phys. 41*, 3088 (1970).]

From 2017 ECE 5390 (Sayak) From paper