SOLUTIONS: ECE 656 Homework 2 (Weeks 3 and 4)

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1) Let $\upsilon(\vec{p})E(\vec{p})$ be the magnitude of the "energy flux" of a beam of electrons with initial momentum, $\vec{p} = p_z\hat{z}$. Write down an expression for the energy flux relaxation time.

Solution:

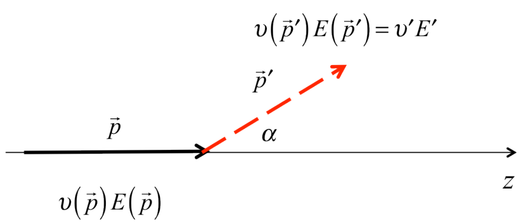
By analogy with the momentum and energy relaxation rates, we write:

$$\frac{1}{\tau_{F_E}} = \sum_{\vec{p}'} S(\vec{p} \to \vec{p}')\frac{\Delta F_E}{F_E} = \sum_{\vec{p}'} S(\vec{p} \to \vec{p}')\frac{F_E(\vec{p}) - F_E(\vec{p}')}{F_E(\vec{p})}$$

$$F_E(\vec{p}) = \vec{\upsilon}(\vec{p})E(\vec{p})$$

$$\boxed{\frac{1}{\tau_{F_E}} = \sum_{\vec{p}'} S(\vec{p} \to \vec{p}')\left[1 - \frac{\upsilon' E'}{\upsilon E}\cos\alpha\right]}$$

where we have aligned the z-axis with the initial flux as shown below.



2) Assume that we have two independent scattering mechanisms, "one" and "two". What is the average time between collisions?

Solution:

The total probability of making a transition from $\vec{p}$ to $\vec{p}'$ is the sum of the probabilities of doing so by the two different mechanisms:

$$S_{TOT}(\vec{p} \to \vec{p}') = S_1(\vec{p} \to \vec{p}') + S_2(\vec{p} \to \vec{p}')$$

ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

The total scattering rate is:

$$\frac{1}{\tau_{TOT}} = \sum_{\vec{p}'} S_{TOT}\left(\vec{p} \to \vec{p}'\right) = \left\{ \sum_{\vec{p}'} S_1\left(\vec{p} \to \vec{p}'\right) + S_2\left(\vec{p} \to \vec{p}'\right) \right\} = \frac{1}{\tau_1} + \frac{1}{\tau_2}$$

So we add scattering **rates**, not scattering times:

$$\boxed{\frac{1}{\tau_{TOT}} = \frac{1}{\tau_1} + \frac{1}{\tau_2}}$$

This result only assumes that the two scattering mechanisms are independent. It is sometimes called **Matthiessen's Rule**, but I don't believe that's correct. Matthiessen's rule states that the total one over the total mobility (or one over the total resistivity) is obtained by adding the reciprocals of the individual components. Resistivity and mobility involve integrating scattering times over energy, and this may not be true – even if the scattering mechanisms are independent.

3) For high energy electrons in semiconductors, the scattering rate may be on the order of 10^{14} per sec. Estimate the collisional broadening. ΔE.

Solution:

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t} = \frac{\hbar}{2\tau} = \frac{\left(1.054\times 10^{-34}\text{ J-s}\right)}{2\times\left(10^{-14}\text{ s}\right)} = 0.53\times 10^{-20} \text{ J}$$

$$\Delta E \geq \frac{0.53\times 10^{-20}}{1.6\times 10^{-19}} \text{ eV} = 0.033 \text{ eV}$$

$$\boxed{\Delta E \geq 0.033 \text{ eV}}$$

4) In Lecture 5 (Lec. 21 from 2011), we worked out the scattering rate for 3D electrons with a short-range scattering potential of $U_S\left(\vec{r}\right) = C\delta\left(0\right)$. Repeat the calculations for 2D electrons with a short-range scattering potential.

Solution:

$$S\left(\vec{p}, \vec{p}'\right) = \frac{2\pi}{\hbar}\left|H_{p',p}\right|^2 \delta\left(E' - E - \Delta E\right) \text{ elastic scattering so } \Delta E = 0$$

ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{p',p}\right|^2 \delta(E'-E)$$

Need to work out the matrix element:

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r})\psi_i d\vec{r}$$

Neglect Bloch functions and assume that the wavefunctions are plane waves:

Initial state and final states:

$$\psi_i = \frac{1}{\sqrt{A}} e^{i\vec{p}\bullet\vec{\rho}/\hbar} \qquad \psi_f = \frac{1}{\sqrt{A}} e^{i\vec{p}'\bullet\vec{\rho}/\hbar}$$

The factor, $1/\sqrt{A}$ is to normalize the wave functions in an area, *A*, and $\vec{\rho}$ is a vector in the *x*-*y* plane. The scattering potential is:

$$U_S(\vec{\rho}) = C\delta(0)$$

The matrix element becomes

$$H_{p',p} = \frac{1}{A}\int_{-\infty}^{+\infty} e^{-i\vec{p}'\bullet\vec{\rho}/\hbar} C\delta(0) e^{i\vec{p}\bullet\vec{\rho}/\hbar} d\vec{\rho} = \frac{C}{A} \ ,$$

and the transition rate becomes

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\frac{C^2}{A^2}\delta(E'-E) = \left(\frac{2\pi C^2}{\hbar A}\right)\frac{1}{A}\delta(E'-E)$$

$$\frac{1}{\tau(\vec{p})} = \sum_{\vec{p}'} S(\vec{p},\vec{p}\,') = \left(\frac{2\pi C^2}{\hbar A}\right)\frac{1}{A}\sum_{\vec{p}'}\delta(E'-E) = \left(\frac{2\pi C^2}{\hbar A}\right)\frac{D_{2D}(E)}{2}$$

so

$\boxed{\dfrac{1}{\tau(E)} \propto D_{2D}(E)}$ as expected.

Note that for any physical problem, we must have $C^2 \propto A$, because the arbitrary normalization area, *A*, must not appear in the final answer.

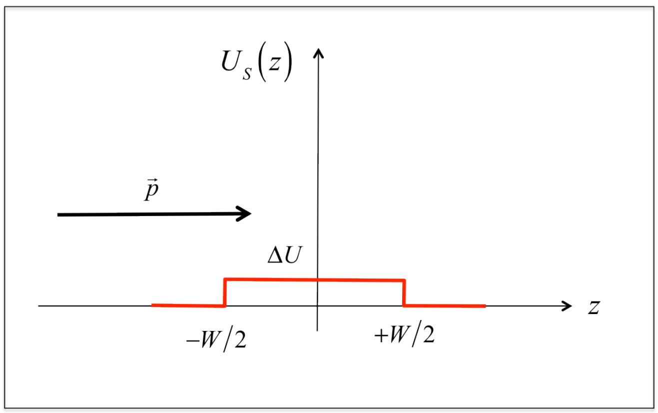
ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

5) Assume a **small** scattering potential as shown below and assume that electrons are free to move only in the z-direction.

a) Work out an expression for the transition rate, $S(\vec{p} \to \vec{p}\,')$, for 1D electrons using Fermi's Golden Rule. Be sure to normalize the wavefunction over a length, L_z.

b) An incident electron with crystal momentum, $\vec{p}$, can only make a transition to one different state, $\vec{p}\,'$. What is that state?

c) Explain what would happen if the sign of ΔU were to change.



Solution:

a)

Matrix element:

$$H_{p',p} = \int_{-W/2}^{+W/2} \frac{e^{-ik_z'z}}{\sqrt{L_z}} \Delta U \frac{e^{ik_z z}}{\sqrt{L_z}} dz$$

$$H_{p',p} = \frac{\Delta U}{L_z} \int_{-W/2}^{+W/2} e^{i(k_z - k_z')z} dz = \frac{2\Delta U}{L_z} \frac{\sin\left(k_z - k_z'\right)W/2}{\left(k_z - k_z'\right)} = \frac{\Delta U W}{L_z}\left(\frac{\sin x}{x}\right)$$

where

$$x = \left(k_z - k_z'\right)W/2$$

$$S(\vec{p},\vec{p}\,') = \frac{2\pi}{\hbar}\left|H_{p',p}\right|^2 \delta\left(E' - E - \Delta E\right) \qquad \text{(elastic scattering so } \Delta E = 0\text{)}$$

ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

$$\boxed{\begin{aligned}&S(\vec{p},\vec{p}\,')=\frac{2\pi}{\hbar}\Delta U^2\left(\frac{W}{L_z}\right)^2\left(\frac{\sin x}{x}\right)^2\delta(E'-E)\\&x=(p_z-p_z')W/2\hbar\end{aligned}}$$

b) There are only two possibilities for elastic scattering in 1D.

case i)

$k_z' = k_z, \quad x = 0 \quad \sin x/x \to 1$

but in this case, the the electron did not scatter – it leaves in the same state it came in.

case ii)

$$\boxed{k_z' = -k_z}$$

Then

$x = (k_z - k_z')W/2 = 2k_zW/2 = k_zW$ and the electron has backscattered.

The transition rate is:

$$S(k_z,-k_z)=\frac{2\pi}{\hbar}\Delta U^2\left(\frac{W}{L_z}\right)^2\left(\frac{\sin k_zW}{k_zW}\right)^2\delta(E'-E)$$

This is the probability of back-scattering.

c)

Let $\Delta U \to -\Delta U$

In this case, we would have a quantum well instead of a quantum barrier. There could be a bound state for electrons in the well. According to FGR, **there would be no difference in the scattering rate.** This is a limitation of FGR; more sophisticated treatments of scattering would show that scattering is stronger when the potential is attractive for the electron. Because of this, the mobility of electrons in n-type material (attractive interaction between the electron and an ionized donor) is less than the minority carrier mobility of electrons in p-type material (repulsive interaction of the electron and ionized acceptor).

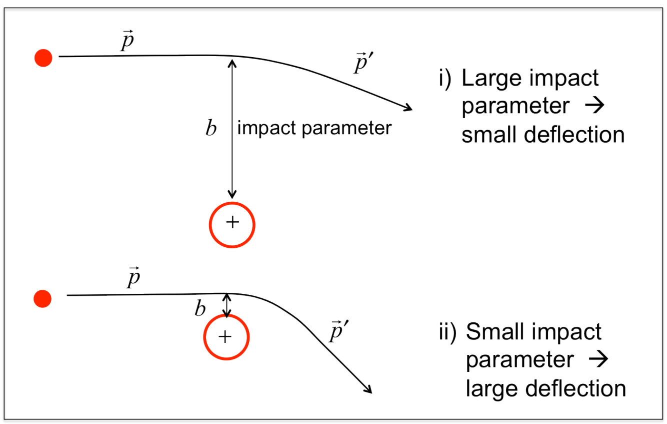
ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

Note: This is a problem that we could solve exactly without Fermi's Golden Rule, which assumes that ΔU is small. Just match the wavefunction and its derivative at $x = -W/2$ and $x = +W/2$.

6) For unscreened Coulomb scattering, the transition rate, $S\left(\vec{p} \to \vec{p}\,'\right)$, goes to infinity for small scattering angles. Explain why this occurs physically. Also explain in words how Conwell and Weisskopf avoid the singularity when integrating the transition rate.

Solution:
As shown below, the further the electron is from the charged impurity, the less it is deflected. The unscreened Coulomb potential, $U_S(r) = q^2 / \left(4\pi\kappa_S\varepsilon_0 r\right)$, is felt to infinite distances, so there is an infinite probability of being deflected (scattered) at an infinitesimally small angle.

Conwell and Weisskopf argued that once an electron is more than half the average distance between impurities away from the impurity in question, then it is closer to another impurity, so there is a minimum angle of deflection. We never let the angle go to zero, so the infinity does not occur.



7) Answer the following questions about Conwell-Weisskopf scattering.

a) Show that the Conwell-Weisskopf scattering rate is

$$\frac{1}{\tau\left(E - E_C\right)} = N_I \pi b_{\max}^2 \frac{\sqrt{2m^*\left(E - E_C\right)}}{m^*}$$

You may assume that $E_C = 0$

ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

b) Provide a simple, physical explanation for the Conwell-Weisskopf scattering rate in terms of the cross-section for scattering, $\pi b_{\max}^2$.

c) Evaluate and plot the scattering rate for electrons in GaAs with the thermal average energy. Compare the scattering rate with the momentum relaxation rate. You should plot τ_m/τ vs. N_I for $10^{14} < N_I < 10^{18}$ cm^{-3}. Explain in physical terms why τ_m and τ differ, and explain why the ratio, τ_m/τ decreases with N_I.

Solution:

a)
This takes a little math…

Equation (2.36) of *Fundamentals of Carrier Transport* (FCT) gives:

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\frac{N_I q^4}{\kappa_S^2\varepsilon_0^2}\frac{1}{\Omega}\sum_{\vec{p},\uparrow}\frac{\delta\left(E-E'\right)}{16\left(p/\hbar\right)^4\sin^2\left(\alpha/2\right)}$$

$$\sin^2\left(\alpha/2\right) = \frac{1}{2}\left(1-\cos\alpha\right) = \frac{1}{2}\left(1-\cos\theta\right) \qquad \left(\theta=\alpha\right)$$

Note that α is the polar angle between the incident momentum and the scattered momentum and θ is the polar angle in our 3D coordinate system. We have simply chosen our z-axis to lie along the direction of the incident momentum, so that $\alpha = \theta$.

We now convert the summation to an integral (remember not to include the factor of 2 for spin!) and find the scattering rate as

$$\frac{1}{\tau} = \frac{2\pi}{\hbar}\frac{N_I q^4}{\kappa_S^2\varepsilon_0^2}\frac{1}{\Omega}\frac{\Omega}{8\pi\hbar^3}\int_0^{2\pi}d\phi\int_{-1}^{\cos\theta_{\min}}\frac{d\left(\cos\theta\right)}{\left(1-\cos\theta\right)^2}\left(\frac{\hbar^4}{16\times\frac{1}{4}p^4}\right)\int_0^{\infty}\delta\left(E-E'\right)p'^2\,dp'$$

$$\frac{1}{\tau} = \frac{N_I q^4}{8\pi\kappa_S^2\varepsilon_0^2 p^4} I_1 \times I_2 \qquad (*)$$

Let $x = \left(1-\cos\theta\right)$

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$$I_1 = \int_{-1}^{\cos\theta_{\min}} \frac{d(\cos\theta)}{(1-\cos\theta)^2} = \int_{2}^{1-\cos\theta_{\min}} \frac{-dx}{x^2} = \frac{1}{1-\cos\theta_{\min}} - \frac{1}{2} = \frac{1}{2}\left(\frac{1}{\sin^2(\theta_{\min}/2)} - 1\right)$$

$$I_1 = \gamma_{CW}^2 / 2 \qquad (**)$$

This is eqn. (2.43) of FCT.

$$I_2 = \int_0^\infty \delta(E - E') p'^2 \, dp'$$

Change variables: $\frac{p'^2}{2m^*} = E' \qquad p'^2 dp' = \sqrt{2}\left(m^*\right)^{3/2}\sqrt{E'}$

Integral 2 becomes

$$I_2 = \int_0^\infty \delta(E - E') p'^2 \, dp' = \sqrt{2}\left(m^*\right)^{3/2}\sqrt{E} \qquad (***)$$

Now use (**) and (***) in (*) to find

$$\frac{1}{\tau} = \frac{N_I q^4}{8\pi\kappa_S^2 \varepsilon_0^2 p^4} \frac{\gamma_{CW}^2}{2} \sqrt{2}\left(m^*\right)^{3/2}\sqrt{E}$$

Finally, use eqn. (2.44) in FCT for $\gamma_{CW}^2/2$ to find:

$$\frac{1}{\tau} = N_I \left(\pi b_{\max}\right)^2 \sqrt{2E/m^*}$$

or

$$\boxed{\frac{1}{\tau} = N_I \left(\pi b_{\max}\right)^2 \upsilon}$$

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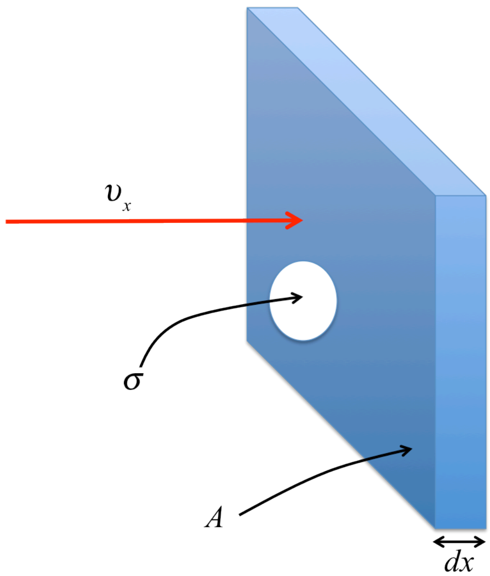
b)

Here, we must recall the concept of "scattering cross section." As shown in the figure below, we think of each scatterer as having an area, σ cm^2.



A beam of electrons is incident on a slab of material with thickness, dx. If N_I is the density of scattering centers (impurities) in the slab (per cm^3), then the number of scatterers in the slab is:

$$num = N_I A dx$$

The fraction of the cross-sectional area obscured by the scatterers is:

$$f = \frac{\sigma N_I A dx}{A} = \sigma N_I dx$$

The probability of scattering in a time, dt, is the scattering rate, $1/\tau$, times dt and is equal to the fraction of the cross-sectional area, A, obscured by the scatterers.

$$\frac{1}{\tau} dt = N_I \sigma dx$$

or

$$\frac{1}{\tau} = N_I \sigma \frac{dx}{dt} = N_I \sigma \upsilon_x$$

ECE 656 Homework 2 (Weeks 3-4) Solutions (continued)

So the scattering rate is proportional to the density of scattering centers, to the cross-sectional area of each scattering center, and to the velocity of electrons (the faster they go, the more scatterers then encounter).

Comparing to the answer in part a), we see that

$$\boxed{\frac{1}{\tau} = N_I \sigma \upsilon \quad \sigma = \pi b_{\max}^2}$$

c)

Use eqn. (2.46) in FCT for the momentum relaxation time and the result it part a) for the scattering time to write:

$$\frac{\tau_m}{\tau} = \left(\frac{4\pi\kappa_S \varepsilon_0 E}{q^2}\right)^2 b_{\max}^2 \frac{1}{\ln\left(1+\gamma_{CW}^2\right)}$$

Assume room temperature, thermal average electrons with $E = 3k_B T/2$, and compute the numbers.

N_I (cm^{-3})	B_{max} (nm)	γ_{CW}	τ_m/τ
10^{14}	110	75	326
10^{15}	50	35	85
10^{16}	23	16	24
10^{17}	11	7.5	7
10^{18}	5	3.5	2.4

We find that $\tau_m > \tau$ because II scattering favors deflections by a small angle.

As the density of impurities increases, $\tau_m \to \tau$. This occurs because $b_{\max}$ decreases, which increases $\theta_{\min}$, so there are fewer and fewer of the small angle deflections, which increase the momentum relaxation time.

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8) Compute and compare the momentum relaxation times due to ionized impurity scattering under the following two circumstances. (Assume GaAs at T_L = 300 K and doped at $N_D = 10^{18}$ cm^{-3}.)

    a) Find $1/\tau_m$ for electrons the thermal average energy, $3k_B T_L/2$.

    b) Find $1/\tau_m$ for electrons the $E = 0.3$ eV. Such electrons can be produced by the heterojunction launching ramp shown in Fig. 3.2 of *Fundamentals of Carrier Transport*.

Solution:

a) $E = 3k_B T/2 = 0.039\ \text{eV}$

Let's first compute the Debye length:

$$L_D = \sqrt{\frac{\kappa_S \varepsilon_0 k_B T}{q^2 n_0}} \quad n_0 = 10^{18}\text{cm}^{-3} \rightarrow L_D = 4.3\ \text{ nm}$$

now compute b_{max}:

$$b_{\max} = \frac{1}{2} N_I^{-1/3} = 0.5\times 10^{-6}\ \text{ cm} = 5\ \text{ nm}$$

The two are so close, that it is not really clear whether to use Conwell-Weisskopf or Brooks-Herring. We'll use Brooks-Herring and compare to Conwell-Weisskopf. From (2.39) in FCT:

$$\gamma^2 = 8m^* E L_D^2 / \hbar^2 = 5.0$$

$$\left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]^{-1} = 1.0$$

From (2.40) FCT, we find:

$$\tau_m = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]^{-1} E^{3/2} = 0.2\ \text{ps}\ \ \text{(The C-W approach gives 0.1 ps)}$$

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b) $E = 0.30\ \text{eV}$

$$\gamma^2 = 8m^* E L_D^2 / \hbar^2 = 39 \qquad \left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]^{-1} = 0.4$$

$$\tau_m = \frac{16\sqrt{2m^*}\pi\kappa_S^2\varepsilon_0^2}{N_I q^4}\left[\ln\left(1+\gamma^2\right) - \frac{\gamma^2}{1+\gamma^2}\right]^{-1} E^{3/2} = 1.5\ \text{ps} \ \ \text{(CW approach gives 0.5 ps)}$$

High-energy carriers are deflected less by ionized impurities than low energy carriers. Depending on whether we use the BH or CW approach, the increase in momentum relaxation time for high energies is a factor of 5 or 7.5.

9) Repeat the electron-phonon energy-momentum conservation arguments discussed in Sec. 2.5 of *Fundamentals of Carrier Transport* and in Lecture 9 (Lec. 25 from 2011), but this time assume electrons in graphene.

Solution:

Begin with energy and momentum conservation:

$$E' = E \pm \hbar\omega \qquad (*)$$
$$\vec{p}\,' = \vec{p} \pm \hbar\vec{\beta} \qquad (**)$$

Use the dispersion of graphene to write:

$$E = \hbar\upsilon_F k = \upsilon_F p$$

$$E^2 = \left(\upsilon_F p\right)^2$$

$$E = \frac{p^2}{\left(E/\upsilon_F^2\right)} = \frac{p^2}{m^*\left(E\right)} \qquad m^*\left(E\right) \equiv \left(E/\upsilon_F^2\right)$$

Using this definition of an effective mass for graphene, (*) becomes

$$\frac{p'^2}{m^*} = \frac{p^2}{m^*} \pm \hbar\omega \qquad (*')$$

which is similar to the parabolic band result.

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Now take the dot product of (**) with itself to find:

$$\vec{p}\,' \bullet \vec{p}\,' = p'^2 = p^2 \pm 2\hbar\vec{p} \bullet \vec{\beta} + \hbar^2\beta^2$$

now divide through by m^*

$$\frac{p'^2}{m^*} = \frac{p^2}{m^*} \pm \frac{2\hbar\vec{p} \bullet \vec{\beta}}{m^*} + \frac{\hbar^2\beta^2}{m^*}$$

and use (*')

$$\pm\hbar\omega = \pm\frac{2\hbar\vec{p} \bullet \vec{\beta}}{m^*} + \frac{\hbar^2\beta^2}{m^*} = \pm\frac{2\hbar p\beta\cos\theta}{m^*} + \frac{\hbar^2\beta^2}{m^*}$$

Solving for $\hbar^2\beta^2 / m^*$ we find

$$\frac{\hbar^2\beta^2}{m^*} = \mp\frac{2\hbar p\beta\cos\theta}{m^*} \pm \hbar\omega$$

$$\hbar\beta = 2p\left[\mp\cos\theta \pm \frac{m^*\omega}{2p\beta}\right],$$

which is a statement of energy and momentum conservation on graphene.

Now use the dispersion of graphene and our definition of effective mass to write

$$\frac{m^*}{p} = \frac{E/\upsilon_F^2}{E/\upsilon_F} = \frac{1}{\upsilon_F}$$

which can be used to express our relation for energy-momentum conservation as

$$\boxed{\hbar\beta = 2p\left[\mp\cos\theta \pm \frac{\omega}{2\beta\upsilon_F}\right]}$$

Note that this result is almost the same as for the parabolic band result (except for the factor of 2 downstairs). The conclusions will be similar.

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10) Assume a transition rate of the form:

$$S\left(\vec{p} \to \vec{p}'\right) = C\,\delta\left(E - E'\right)\delta_{\vec{p}',\vec{p}\pm\hbar\beta}$$

where C is a constant. Answer the following questions assuming parabolic energy bands.

a) Derive an expression for $\left|\vec{\beta}\right|$, which expresses conservation of energy and momentum.
b) Using the results of a), determine the minimum and maximum magnitude of $\left|\vec{\beta}\right|$.

Solution:

a)

Begin with energy and momentum conservation:

$$E' = E \qquad (*)$$
$$\vec{p}' = \vec{p} \pm \hbar\vec{\beta} \qquad (**)$$

Since the band are parabolic, (*) can be written as:

$$\frac{p'^2}{2m^*} = \frac{p^2}{2m^*} \pm \hbar\omega \qquad (*')$$

Now take the dot product of (**) with itself to find:

$$\vec{p}' \bullet \vec{p}' = p'^2 = p^2 \pm 2\hbar\vec{p} \bullet \vec{\beta} + \hbar^2\beta^2$$

now divide through by $2m^*$

$$\frac{p'^2}{2m^*} = \frac{p^2}{2m^*} \pm \frac{2\hbar\vec{p} \bullet \vec{\beta}}{2m^*} + \frac{\hbar^2\beta^2}{2m^*}$$

and use (*')

$$\frac{p'^2}{2m^*} - \frac{p^2}{2m^*} = 0 = \pm\frac{2\hbar\vec{p} \bullet \vec{\beta}}{2m^*} + \frac{\hbar^2\beta^2}{2m^*} = \pm\frac{2\hbar p\beta\cos\theta}{2m^*} + \frac{\hbar^2\beta^2}{2m^*}$$

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Solving for $\hbar\beta$ we find

$\boxed{\hbar\beta = \mp 2p\cos\theta}$,

which is a statement of energy and momentum conservation on for elastic scattering.

b)

Note that β is the magnitude of $\vec{\beta}$, so it must always be greater than or equal to zero.

The largest β will occur for

Absorption: $\cos\theta = -1, \quad \theta = \pi$
Emission: $\cos\theta = 1, \quad \theta = 0$

In either case, $\hbar\beta_{\max} = 2p$

The smallest β occurs for $\theta = \pi/2$ for both absorption and emission.

In either case, $\hbar\beta_{\min} = 0$

We conclude that for elastic scattering:

$\boxed{0 \le \hbar\beta \le 2p}$