Side notes:

In here, we will derive the general expressions for the calculation of the scattering rates out of some initial state k. We will consider two cases, most often found when calculating the scattering rates for arbitrary scattering potential:

(a) δ-function perturbation for which the matrix element $V(\vec{q}) = V_0 = \text{const}$.

(b) Matrix element $V(\vec{q})$ which is a function of $\vec{q} = \vec{k} - \vec{k}'$ (momentum transfer in the scattering process).

(a) Constant matrix element:

$$S(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar} |V_0|^2 \delta(E_{k'} - E_k \pm \hbar\omega_0)$$

The total scattering rate out of a state $\vec{k}$ is then given by:

$$\frac{1}{\tau(\vec{k})} = \sum_{\vec{k}'} S(\vec{k}, \vec{k}') = \frac{2\pi |V_0|^2}{\hbar} \frac{\Omega}{(2\pi)^3} \int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} k'^2 dk' \, \delta(E_{k'} - E_k \pm \hbar\omega_0)$$

If we assume parabolic energy bands, then:

$$E_{k'} = \frac{\hbar^2 k'^2}{2m^*}$$

which leads to:

$$k' = \sqrt{\frac{2m^* E_{k'}}{\hbar^2}} \quad \text{and} \quad k' dk' = \frac{m^*}{\hbar^2} dE_{k'}$$

Substituting these results into the expression $1/\tau(\vec{k})$ gives:

$$\frac{1}{\tau(k)} = \frac{2\pi}{\hbar} |V_0|^2 \frac{\Omega}{(2\pi)^3} \cdot 4\pi \, \frac{m^*}{\hbar^2} \sqrt{\frac{2m^*}{\hbar^2}} \int_0^{\infty} dE_{k'} \sqrt{E_{k'}} \, \delta(E_{k'} - E_k \pm \hbar\omega_0)$$

$$= \frac{2\pi}{\hbar} |V_0|^2 \frac{\Omega}{2\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{3/2} \frac{1}{2} \sqrt{E_k \mp \hbar\omega_0} = \frac{2\pi}{\hbar} |V_0|^2 \frac{1}{2} g_c(E_k \mp \hbar\omega_0)$$

$\frac{1}{2}$ comes from the fact that the scattering process is assumed not to flip the spin of the electron, which means that only half of the total # of final states is available.

- This model matrix element is important when considering acoustic phonon scattering in the elastic and equipartition approximation.

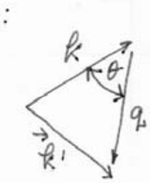
(b) Momentum dependent matrix element

- We now consider the general case of a momentum dependent matrix element as it occurs, for example, in general description of phonon scattering. The transition rate from some initial state $\vec{k}$ to some final state $\vec{k}'$ is, in general, given by:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\,|M(\vec{k},\vec{q})|^2\,\underbrace{\delta(E_{k'} - E_k \overset{\text{emission}}{\underset{\text{abs.}}{\pm}} \hbar\omega_0)}_{\substack{\text{energy conservation}\\ \text{satisfied only in the}\\ \text{long-time limit.}}}\;\underbrace{\delta(\vec{k}' - \vec{k} \pm \vec{q})}_{\substack{\text{momentum conservation}\\ \text{is always satisfied}}}$$

From the momentum conservation we have:

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



which gives:

$$E_{k'} - E_k \pm \hbar\omega_0 = \frac{\hbar^2}{2m^*}k'^2 - \frac{\hbar^2}{2m^*}k^2 \pm \hbar\omega_0$$

$$= \frac{\hbar^2}{2m^*}\left[\cancel{k^2} + q^2 \mp 2kq\cos\theta\right] - \cancel{\frac{\hbar^2 k^2}{2m^*}} \pm \hbar\omega_0$$

$$= \frac{\hbar^2}{2m^*}\left(q^2 \mp 2kq\cos\theta \pm \frac{2m^*}{\hbar^2}\hbar\omega_0\right)$$

$$= \frac{\hbar^2}{2m^*}\left(q^2 \mp 2kq\cos\theta \pm \frac{2m^*\hbar\omega_0}{\hbar\cancel{^2}}\right)$$

$$= \frac{\hbar^2}{\cancel{2}m^*}\cancel{2}kq\left[\frac{q^{\cancel{2}}}{2k\cancel{q}} \mp \cos\theta \pm \frac{\cancel{2}m^*\omega_0}{\hbar\cdot\cancel{2}kq}\right]$$

$$= \frac{\hbar^2 kq}{m^*}\left[\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega_0}{\hbar kq}\right]$$

Using the following relationship:

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

we arrive at the following expression for $S(\vec{k},\vec{k}')$:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\,|M(\vec{k},\vec{q})|^2 \frac{m^*}{\hbar^2 kq}\,\delta\left(\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq}\right)$$

- Because of the energy conservation requirement, the magnitude of the momentum transfer in the scattering process (phonon wavevector) and the angle θ are not independent, and their relationship is derived by setting the argument of the δ-function to zero, i.e.

$$\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq} = 0$$

Depending upon the variation of ω_q, this will give different minimum and maximum values of q.

- The integral over all possible values of k' (possible final states) is equivalent to the one that takes into account all possible momentum transfers in the scattering process. Therefore, the scattering rate out of some initial state $\vec{k}$ can be evaluated using:

$$\frac{1}{\tau(k)} = \sum_q \frac{2\pi}{\hbar}|M(\vec{k},\vec{q})|^2 \frac{m^*}{\hbar^2 kq}\,\delta\left(\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq}\right)$$

$$= \frac{2\pi}{\hbar}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\int_0^{\infty} \Omega\frac{q^{\cancel{2}}dq}{(2\pi)^3}\,\frac{m^*}{\hbar^2 k\cancel{q}}\,\delta\left(\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq}\right)|M(\vec{k},\vec{q})|^2$$

$$= \frac{(2\pi)^2 m^*\Omega}{(2\pi)^3\hbar^3 k}\int_0^{\infty} q\,dq \int_{-1}^{1} d(\cos\theta)\,\delta\left(\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq}\right)|M(\vec{k},\vec{q})|^2$$

$$= \frac{m^*\Omega}{2\pi\hbar^3 k}\int_{q_{min}}^{q_{max}} q\,|M(\vec{k},\vec{q})|^2\,dq$$

To summarize, for arbitrary matrix element, the total scattering rate out of some initial state is given by:

$$\frac{1}{\tau(\vec{k})} = \frac{m^*\Omega}{2\pi\hbar^3 k}\int_{q_{min}}^{q_{max}} q\,|M(\vec{k},\vec{q})|^2 dq$$

where the limits of the integration (q_{min} and q_{max}) are obtained from:

$$\frac{q}{2k} \mp \cos\theta \pm \frac{m^*\omega}{\hbar kq} = 0$$

Calculation of the scattering rates for arbitrary matrix elements:

$$P(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}|M(\vec{k},\vec{q})|^2\,\delta(E_{k'} - E_k \mp \hbar\omega_q)\ ;\ |M(k,q)|^2 = C_q^2\,\delta(k-k'\pm q)$$

We need to consider two separate cases:

(a) constant matrix element
(b) General q-dependent matrix element

$$\frac{1}{\tau(k)} = \frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta) \int_0^{\infty} q^2 dq\, C_q^2\, \delta(\vec{k}-\vec{k}' \pm \vec{q})\,\delta(E_{k'} - E_k \mp \hbar\omega_q)$$

$$= \frac{V}{2\pi\hbar}\int_{-1}^{1} d(\cos\theta)\int_0^{\infty} q^2 dq\, C_q^2\,\delta(\vec{k}-\vec{k}' \pm \vec{q})\,\delta(E_{k'} - E_k \mp \hbar\omega_q)$$

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

$$\frac{\hbar^2}{2m}(\cancel{k^2} \pm 2kq\cos\theta + q^2) - \cancel{\frac{\hbar^2 k^2}{2m}} \mp \hbar\omega_q = 0$$

$$\pm\frac{\hbar^2}{\cancel{2}m}\cancel{2}kq\cos\theta + \frac{\hbar^2 q^2}{2m} \mp \hbar\omega_q = 0$$

$$\frac{\hbar^2 kq}{m}\cos\theta \pm \frac{\hbar^2 q^2}{2m} - \hbar\omega_q = 0$$

$$\delta(\qquad\qquad) = \frac{m}{\hbar^2 kq}\,\delta\left(\cos\theta \pm \frac{\cancel{m}}{\cancel{\hbar^2} k\cancel{q}}\frac{\cancel{\hbar^2} q^{\cancel{2}}}{2\cancel{m}} - \frac{m}{\hbar^2 kq}\hbar\omega_q\right)$$

$$= \frac{m}{\hbar^2 kq}\,\delta\left(\cos\theta \pm \frac{q}{2k} - \frac{m\omega_q}{\hbar kq}\right)$$

$$\frac{1}{\tau(k)} = \frac{V}{2\pi\hbar}\frac{m}{\hbar^2 k}\int_{q_{min}}^{q_{max}} q^2 dq\,\frac{1}{q}\,C_q^2 = \frac{mV}{2\pi\hbar^3 k}\int_{q_{min}}^{q_{max}} q\,C_q^2\,dq$$