0.1 Expression de τ^{c-LO}

Step 1 Carrier - phonon : From the Fermi Golden Rule to the interaction rate

The Fermi Golden Rule gives the rate of phonons absorption / emission through their interactions with carriers at temperature T. This expressions can be used in a detail balance on phonon populations :

$$\left.\frac{dN_{\mathbf{q}}}{dt}\right)_{c-LO} \simeq \frac{4\pi}{\hbar}|M_{\mathbf{q}}|^2 \sum_{\mathbf{k}} (N_{\mathbf{q}}+1)\ f_{\mathbf{k}}(1-f_{\mathbf{k-q}})\delta\left(E_k - E_{k-q} - \hbar\omega_q\right) \\ - N_{\mathbf{q}} f_{\mathbf{k-q}}(1-f_{\mathbf{k}})\delta\left(E_k - E_{k-q} - \hbar\omega_q\right) \quad (1)$$

where $N_{\mathbf{q}}$ is the actual phonon population of mode $\mathbf{q}$ and $|M_{\mathbf{q}}|^2$ is the interaction matrix element.

To do so, we need to calculate the quantity

$$A = \sum_{\mathbf{k}} (N_{\mathbf{q}}+1)\ f_{\mathbf{k}}(1-f_{\mathbf{k-q}})\delta\left(E_k - E_{k-q} - \hbar\omega_q\right) \\ - N_{\mathbf{q}} f_{\mathbf{k-q}}(1-f_{\mathbf{k}})\delta\left(E_k - E_{k-q} - \hbar\omega_q\right)$$

where the dispersion relation is assumed to be that of free particles

$$\begin{aligned} E_k - E_{k-q} &= \frac{\hbar^2}{2m}\left(k^2 - (k^2 + q^2 - 2\mathbf{k}.\mathbf{q})\right) \\ &= \frac{\hbar^2}{m} kq\cos\theta - \frac{\hbar^2 q^2}{2m} \end{aligned}$$

and we define θ in the spherical coordinates by taking the z-axis along $\mathbf{q}$.

We change the sum to an integral using the density of state

$$\sum_{\mathbf{k}} \to \int d^3\mathbf{k}\, \rho(\mathbf{k}) = \left(\frac{L}{2\pi}\right)^3 \int d^3\mathbf{k}$$

hence

$$\begin{aligned} A =& \frac{L^3}{8\pi^3} \int k^2 dk \sin\theta d\theta d\varphi \left[(N_{\mathbf{q}}+1)\ f_{\mathbf{k}}(1-f_{\mathbf{k-q}}) - N_{\mathbf{q}} f_{\mathbf{k-q}}(1-f_{\mathbf{k}})\right] \\ &\times \delta\left(\frac{\hbar^2}{m} kq\cos\theta - \frac{\hbar^2 q^2}{2m} - \hbar\omega_q\right) \\ =& \frac{L^3}{8\pi^3} 2\pi \int_0^\infty k^2 dk \int_{-1}^{1} d(\cos\theta)\, \frac{m}{\hbar^2 kq} \left[(N_{\mathbf{q}}+1)\ f_{\mathbf{k}}(1-f_{\mathbf{k-q}}) - N_{\mathbf{q}} f_{\mathbf{k-q}}(1-f_{\mathbf{k}})\right] \\ &\times \delta\left(\cos\theta - \frac{1}{k}\left(\frac{q}{2} + \frac{m\omega_q}{\hbar q}\right)\right) \end{aligned}$$

where we used $\delta(\alpha x) = \alpha^{-1}\delta(x)$. The delta function will keep only a single value of θ such that $\cos\theta = \frac{1}{k}(\frac{q}{2} + \frac{m\omega_q}{\hbar q})$ - which is only possible if $k \geq \frac{q}{2} + \frac{m\omega_q}{\hbar q} = k_{\min}$; and for this specific value of θ, $E_{\mathbf{k-q}} = \frac{\hbar^2}{2m}\left(k^2 + q^2 - 2kq\cos\theta\right) = \frac{\hbar^2 k^2}{2m} - \hbar\omega_{\mathbf{q}}$. As a result, $f_{\mathbf{k-q}}$ takes value

$$f_{\mathbf{k-q}} \to \frac{1}{\exp\left(\frac{E_k}{k_B T} - \frac{\hbar\omega_q}{k_B T} - \frac{\mu_n}{k_B T}\right) + 1} = f_{\epsilon_k - \epsilon_{\mathbf{q}}}$$

where we note $\epsilon_k = E_k/kT$ and $\epsilon_q = \hbar\omega_q/kT$. By contrast, $f_{\mathbf{k}} = f_{\epsilon_k}$ is independent of θ and can be taken out of the integral over θ. We have therefore

$$
\begin{aligned}
A =& \frac{mL^3}{4\hbar^2 q\pi^2}\int_{k_{\min}}^{\infty} kdk\left[\left(N_q+1\right)\, f_{\epsilon_k}(1-f_{\epsilon_k-\epsilon_{\mathbf{q}}}) - N_q\, f_{\epsilon_k-\epsilon_{\mathbf{q}}}(1-f_{\epsilon_k})\right]\\
=& \frac{mL^3}{4\hbar^2 q\pi^2}\int_{k_{\min}}^{\infty} kdk\left[f_{\epsilon_k}(1-f_{\epsilon_k-\epsilon_{\mathbf{q}}}) - N_q\left(f_{\epsilon_k-\epsilon_{\mathbf{q}}}-f_{\epsilon_k}\right)\right]\\
=& \frac{m^2L^3k_BT}{4\hbar^4 q\pi^2}\int_{\epsilon_{\min}}^{\infty} d\epsilon\left[f_{\epsilon}(1-f_{\epsilon-\epsilon_{\mathbf{q}}}) - N_q\left(f_{\epsilon-\epsilon_{\mathbf{q}}}-f_{\epsilon}\right)\right]
\end{aligned}
$$

where we used the variable change $\epsilon = \frac{1}{k_BT}\frac{\hbar^2k^2}{2m} \to kdk = \frac{mk_BT}{\hbar^2}d\epsilon$. Finally, using the same trick as Wurfel's derivation of the GPL, we express:

$$
\begin{aligned}
f_{\epsilon_k}(1-f_{\epsilon_k-\epsilon_{\mathbf{q}}}) =& \frac{f_{\epsilon_k}(1-f_{\epsilon_k-\epsilon_{\mathbf{q}}})}{f_{\epsilon_k-\epsilon_{\mathbf{q}}}-f_{\epsilon_k}}\times\left(f_{\epsilon_k-\epsilon_{\mathbf{q}}}-f_{\epsilon_k}\right)\\
=& \frac{1}{e^{\frac{\hbar\omega_{\mathbf{q}}}{k_BT}}-1}\times\left(f_{\epsilon_k-\epsilon_{\mathbf{q}}}-f_{\epsilon_k}\right)
\end{aligned}
$$

where we recognize $\left(e^{\hbar\omega_{\mathbf{q}}}-1\right)^{-1}$ as the thermal occupation factor $N_{\mathbf{q}}(T)$. We can finally conclude from eq. 1 to get

$$
\begin{aligned}
\left.\frac{dN_{\mathbf{q}}}{dt}\right)_{c-LO} \simeq& \left(N_{\mathbf{q}}(T)-N_{\mathbf{q}}\right)\times 2\times\frac{2\pi}{\hbar}|M_{\mathbf{q}}|^2\frac{m^2L^3k_BT}{4\hbar^4q\pi^2}\int_{\epsilon_{\min}}^{\infty} d\epsilon\, f_{\epsilon-\epsilon_{\mathbf{q}}}-f_{\epsilon}\\
=& \frac{N_{\mathbf{q}}(T)-N_{\mathbf{q}}}{\tau}
\end{aligned}
$$

with

$$
\begin{aligned}
\frac{1}{\tau} &= |M_{\mathbf{q}}|^2\frac{m^2L^3k_BT}{\hbar^5q\pi}\int_{0}^{\infty} d\epsilon\, f_{\epsilon+\epsilon_{\min}-\epsilon_{\mathbf{q}}}-f_{\epsilon+\epsilon_{\min}}\\
&= |M_{\mathbf{q}}|^2\frac{m^2L^3k_BT}{\hbar^5q\pi}\,\ln\left(\frac{\exp\left(\frac{E_{\min}-\mu}{kT}\right)+1}{\exp\left(\frac{E_{\min}-\hbar\omega_{\mathbf{q}}-\mu}{kT}\right)+1}\right)\\
&= |M_{\mathbf{q}}|^2\frac{m^2L^3k_BT}{\hbar^5q\pi}\,\ln\left(\frac{1+\exp\left(-\frac{E_{\min}-\hbar\omega_{\mathbf{q}}-\mu}{kT}\right)}{1+\exp\left(-\frac{E_{\min}-\mu}{kT}\right)}\right)
\end{aligned}
$$

Step 2 Carrier - phonon : Simplify the expression for the interaction rate

Using the expression of $E_{\min} = \frac{\hbar^2}{2m}\left(\frac{q}{2}+\frac{m\omega_q}{\hbar q}\right)^2$, the interaction rate can be expressed as

$$
\frac{1}{\tau} = |M_{\mathbf{q}}|^2\frac{m^2L^3k_BT}{\hbar^5q\pi}\,\ln\left(\frac{1+\exp\left(\frac{\mu}{kT}-\frac{\hbar^2q^2}{8mkT}-\frac{m\omega_q^2}{2q^2kT}+\frac{\hbar\omega_q}{2kT}\right)}{1+\exp\left(\frac{\mu}{kT}-\frac{\hbar^2q^2}{8mkT}-\frac{m\omega_q^2}{2q^2kT}-\frac{\hbar\omega_q}{2kT}\right)}\right) \tag{2}
$$

The expression of the matrix element is

$$
\begin{aligned}
|M_{\mathbf{q}}|^2 &= \frac{1}{L^3} \frac{e^2 \hbar \omega_{\mathbf{q}}}{2\epsilon_0 \left(1 + \frac{q_s^2}{q^2}\right) q^2} \left(\frac{1}{K_\infty} - \frac{1}{K_s} \right) && (3) \\
&\simeq \frac{1}{L^3} \frac{e^2 \hbar \omega_{\mathbf{q}}}{2\epsilon_\infty q^2} \underbrace{\frac{1}{\left(1 + \frac{q_s^2}{q^2}\right)}}_{= \eta_{\text{screening}}} && (4)
\end{aligned}
$$

leading to

$$
\begin{aligned}
\tau &= \frac{2\pi\epsilon_\infty \hbar^4}{e^2 \omega_{\mathbf{q}} m^2} \frac{q^3}{k_B T} \left(1 + \frac{q_s^2}{q^2}\right) \frac{1}{\ln\left(\frac{1+\exp\left(\frac{\mu}{kT} - \frac{\hbar^2 q^2}{8mkT} - \frac{m\omega_q^2}{2q^2 kT} + \frac{\hbar\omega_q}{2kT} \right)}{1+\exp\left(\frac{\mu}{kT} - \frac{\hbar^2 q^2}{8mkT} - \frac{m\omega_q^2}{2q^2 kT} - \frac{\hbar\omega_q}{2kT} \right)} \right)} && (5) \\
&= \frac{2\pi\epsilon_\infty \hbar^4}{e^2 \omega_{\mathbf{q}} m^2} \frac{q^3}{k_B T} \left(1 + \frac{q_s^2}{q^2}\right) \frac{1}{\ln\left(\frac{1+\exp\left(\frac{\mu}{kT} - \frac{1}{4} \frac{\hbar^2 q^2}{2mkT} - \frac{2mkT}{\hbar^2 q^2} \left(\frac{\hbar\omega_q}{2k_B T} \right)^2 + \frac{\hbar\omega_q}{2kT} \right)}{1+\exp\left(\frac{\mu}{kT} - \frac{1}{4} \frac{\hbar^2 q^2}{2mkT} - \frac{2mkT}{\hbar^2 q^2} \left(\frac{\hbar\omega_q}{2k_B T} \right)^2 - \frac{\hbar\omega_q}{2kT} \right)} \right)} && (6) \\
&= \frac{2\pi\epsilon_\infty \hbar}{e^2 \omega_{\mathbf{q}}} \sqrt{\frac{k_B T}{m}} \tilde{q}^3 \left(1 + \frac{\tilde{q}_s^2}{\tilde{q}^2}\right) \frac{1}{\ln\left(\frac{1+\exp\left(\frac{\mu}{kT} - \frac{1}{4} \frac{\hbar^2 q^2}{2mkT} - \frac{2mkT}{\hbar^2 q^2} \left(\frac{\hbar\omega_q}{2k_B T} \right)^2 + \frac{\hbar\omega_q}{2kT} \right)}{1+\exp\left(\frac{\mu}{kT} - \frac{1}{4} \tilde{q}^2 - \frac{1}{\tilde{q}^2} \left(\frac{\hbar\omega_q}{2k_B T} \right)^2 - \frac{\hbar\omega_q}{2kT} \right)} \right)} && (7)
\end{aligned}
$$