

Starting from equation (13) in reference (18), *Size effects in thermal conduction by phonons*:(p=2)

$$\begin{aligned}
\kappa(q) &= \frac{1}{\Omega} \sum_{Q=(\vec{Q},s)} \frac{\hbar \omega_Q v_{Q_x}^2 (\partial n_Q / \partial T)}{1/\tau_Q + i q v_{Q_x}} \\
&= \frac{1}{\Omega} \sum_{Q=(\vec{Q},s)} \frac{k_B v_{Q_x}^2}{1/\tau_Q + i q v_{Q_x}} \\
&= \frac{3}{\Omega} \cdot k_B \sum_{\vec{Q}} \frac{v_{Q_x}^2}{1/\tau_Q + i q v_{Q_x}} \\
&= \frac{3k_B}{\Omega} \sum_{\vec{Q}} \frac{v_{Q_x}^2 \tau_Q}{1 + i q v_{Q_x} \tau_Q} \\
&= \frac{3k_B v^2 \tau_D}{\Omega} \sum_{\vec{Q}} \frac{(\frac{Q_x}{Q})^2 (\frac{Q_D}{Q})^p}{1 + i q v (\frac{Q_x}{Q}) \tau_D (\frac{Q_D}{Q})^p} \\
&= \frac{3k_B v^2 \tau_D}{\Omega} \int_0^{\omega_D} \frac{(\frac{\omega_D}{\omega})^p \cos^2 \theta}{1 + i q v \tau_D (\frac{\omega_D}{\omega})^p \cos \theta} \cdot c(\omega) d\omega \cdot [\frac{1}{2} \int_{-1}^1 d(\cos \theta)] \\
&= \frac{3k_B v^2 \tau_D}{\Omega} \int_0^{\omega_D} (\frac{\omega_D}{\omega})^p \cdot c(\omega) d\omega \cdot [\frac{1}{2} \int_{-1}^1 \frac{\cos^2 \theta}{1 + i q v \tau_D (\frac{\omega_D}{\omega})^p \cos \theta} d(\cos \theta)]
\end{aligned}$$

Let q=0:

$$\begin{aligned}
\kappa_0 = \kappa(0) &= \frac{3k_B v^2 \tau_D}{\Omega} \int_0^{\omega_D} (\frac{\omega_D}{\omega})^p \cdot c(\omega) d\omega \cdot [\frac{1}{2} \int_{-1}^1 \cos^2 \theta d(\cos \theta)] \\
&= \frac{k_B v^2 \tau_D}{\Omega} \int_0^{\omega_D} (\frac{\omega_D}{\omega})^p \cdot c(\omega) d\omega \\
&= \frac{k_B v^2 \tau_D}{\mathcal{V}} \int_0^{\omega_D} (\frac{\omega_D}{\omega})^p \cdot \frac{\mathcal{V} \omega^2}{2\pi^2 v^3} d\omega \\
&\stackrel{p=2}{=} \frac{k_B v^2 \tau_D}{2\pi^2 v^3} \cdot \omega_D^2 \int_0^{\omega_D} d\omega \\
&= \frac{k_B v^2 \tau_D}{2\pi^2 v^3} \cdot \omega_D^3 \\
&= \frac{k_B v^2 \tau_D}{2\pi^2 v^3} \cdot \frac{6\pi^2 N v^3}{\Omega} = \frac{3k_B v^2 \tau_D}{\Omega}
\end{aligned}$$

Back to equation (9) in *2NL.pdf*:

$$\begin{aligned}
\kappa(q) &= \frac{1}{\Omega} \sum_{Q=(\vec{Q},s)} k_B v_{\vec{Q}_x}^2 \tau_Q \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
&= \frac{1}{\Omega} k_B v^2 \tau_D \sum_{Q=(\vec{Q},s)} \left(\frac{Q_x}{Q}\right)^2 \left(\frac{Q_D}{Q}\right)^p \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
&= \frac{N}{\Omega} k_B v^2 \tau_D \cdot \frac{1}{N} \sum_{Q=(\vec{Q},s)} \left(\frac{Q_x}{Q}\right)^2 \left(\frac{Q_D}{Q}\right)^p \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
&= \frac{3N}{\Omega} k_B v^2 \tau_D \times \frac{1}{N} \sum_{\vec{Q}} \left(\frac{Q_x}{Q}\right)^2 \left(\frac{Q_D}{Q}\right)^p \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
&= \kappa_0 \times \frac{1}{N} \sum_{\vec{Q}} \left(\frac{Q_x}{Q}\right)^2 \left(\frac{Q_D}{Q}\right)^p \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
\\
\kappa(q) &= \kappa_0 \times \frac{1}{N} \sum_{\vec{Q}} \left(\frac{Q_x}{Q}\right)^2 \left(\frac{Q_D}{Q}\right)^p \cos^2(qd/2) F(q, \Lambda_{Q_x}) \\
\kappa_0 &= \frac{3N}{\Omega} k_B v^2 \tau_D
\end{aligned}$$

$Q_D = (6\pi^2(N/V))^{1/3}$ in the case of fcc $Q_D = (3/\pi)^{1/3} \frac{2\pi}{a} = 0.985 \frac{2\pi}{a}$
 Q_x is the projection of \vec{Q} in (1,1, $\bar{1}$) direction.