Equations for iterative solution to phonon BTE

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1 The Boltzmann equation for Phonon

We write the Boltzmann equation for phonon as:

$$\frac{\partial n_1}{\partial t} = -\frac{\partial H_1}{\partial p}\frac{\partial n_1}{\partial r} + \left(\frac{\partial n_1}{\partial t}\right)_{coll} = 0 \tag{1}$$

where index 1 indicate single particle distribution function and Hamiltonian. the diffusion part can be written linear to temperature gradient ∇T as:

$$v_{k,s}\frac{\partial n^0_{k,s}}{\partial T}\nabla T = \left(\frac{\partial n_{k,s}}{\partial t}\right)_{coll} = \left(\frac{\partial n_{k,s}}{\partial t}\right)_{3ph} + \left(\frac{\partial n_{k,s}}{\partial t}\right)_{other} \tag{2}$$

for each of the phonon state indexed by (k, s).

2 three phonon scattering and iterative solution

The collision term includes the scattering events that change the phonon distribution at state (k, s). Below we use the notation so that $q_1 = (k_1, s_1); q_2 = (k_2, s_2); q_3 = (k_3, s_3)$. The collision term due to 3 phonon interaction can be written as:

$$\begin{aligned}\left(\frac{\partial n_{q_1}}{\partial t}\right)_{3ph} = \sum_{q_2,q_3}\{ &- n_{q_1}n_{q_2}(n_{q_3}+1)L^{q_3}_{q_1,q_2} + (n_{q_1}+1)(n_{q_2}+1)n_{q_3}L^{q_1,q_2}_{q_3} \\ &+ \frac{1}{2}\left[-n_{q_1}(n_{q_2}+1)(n_{q_3}+1)L^{q_2,q_3}_{q_1} + (n_{q_1}+1)n_{q_2}n_{q_3}L^{q_1}_{q_2,q_3}\right]\}\end{aligned} \tag{3}$$

In the above equation, L^j_i is the transition probability from initial state i to final state j and we have $L^{q_3}_{q_1,q_2} = L^{q_1,q_2}_{q_3}$ and $L^{q_1}_{q_2,q_3} = L^{q_2,q_3}_{q_1}$. $\frac{1}{2}$ in the summation avoid double counting. L^j_i includes the requirement for energy and momentum conservation:

$$L^{q_3}_{q_1,q_2} : \delta(k_1 + k_2 - k_3)\delta(\omega_1 + \omega_2 - \omega_3) \tag{4}$$

$$L^{q_2,q_3}_{q_1} : \delta(k_1 - k_2 - k_3)\delta(\omega_1 - \omega_2 - \omega_3) \tag{5}$$

Now, we write the phonon distribution function n_q as:

$$n_q \approx n^0_q + \beta n^0_q(n^0_q + 1)\Phi_q \tag{6}$$

putting the above equation.6 into equation.3, to the first order in Φ_q we have:

$$\left(\frac{\partial n_{q_1}}{\partial t}\right)_{3ph} = -\beta\sum_{q_2,q_3}\left\{P^{q_3}_{q_1,q_2} + \frac{1}{2}P^{q_2,q_3}_{q_1}\right\} \tag{7}$$

and

$$\begin{aligned}P^{q_3}_{q_1,q_2} = [\ &(n^0_{q_2} - n^0_{q_3})n^0_{q_1}(n^0_{q_1}+1)\Phi_{q_1} + \\ &(n^0_{q_1} - n^0_{q_3})n^0_{q_2}(n^0_{q_2}+1)\Phi_{q_2} - (n^0_{q_1} + n^0_{q_2} + 1)n^0_{q_3}(n^0_{q_3}+1)\Phi_{q_3}]L^{q_3}_{q_1,q_2}\end{aligned} \tag{8}$$

$$\begin{aligned}P^{q_2,q_3}_{q_1} = [\ &(n^0_{q_2} + n^0_{q_3} + 1)n^0_{q_1}(n^0_{q_1}+1)\Phi_{q_1} + \\ &(n^0_{q_1} - n^0_{q_3})n^0_{q_2}(n^0_{q_2}+1)\Phi_{q_2} + (n^0_{q_1} - n^0_{q_2})n^0_{q_3}(n^0_{q_3}+1)\Phi_{q_3}]L^{q_2,q_3}_{q_1}\end{aligned} \tag{9}$$

and it can be shown that when the energy conservation included in the $L^{q_3}_{q_1,q_2}$ and $L^{q_1}_{q_2,q_3}$ are satisfied, the terms including n_q can be simplified:

$$\begin{aligned}
n^0_{q_1} n^0_{q_2} (n^0_{q_3}+1) &= (n^0_{q_2} - n^0_{q_3}) n^0_{q_1} (n^0_{q_1}+1) \\
&= (n^0_{q_1} - n^0_{q_3}) n^0_{q_2} (n^0_{q_2}+1) \\
&= (n^0_{q_1} + n^0_{q_2}+1) n^0_{q_3} (n^0_{q_3}+1) \qquad (10)\\
n^0_{q_1} (n^0_{q_2}+1)(n^0_{q_3}+1) &= (n^0_{q_2} + n^0_{q_3}+1) n^0_{q_1} (n^0_{q_1}+1) \\
&= -(n^0_{q_1} - n^0_{q_3}) n^0_{q_2} (n^0_{q_2}+1) \\
&= -(n^0_{q_1} - n^0_{q_2}) n^0_{q_3} (n^0_{q_3}+1) \qquad (11)
\end{aligned}$$

So equation.9 can be simplified to be:

$$\left(\frac{\partial n_{q_1}}{\partial t}\right)_{3ph} = -\beta \sum_{q_2,q_3} \{ \ (\Phi_{q_1} + \Phi_{q_2} - \Phi_{q_3})\, n^0_{q_1} n^0_{q_2} (n^0_{q_3}+1) L^{q_3}_{q_1,q_2} \qquad (12)$$

$$+\frac{1}{2} (\Phi_{q_1} - \Phi_{q_2} - \Phi_{q_3})\, n^0_{q_1} (n^0_{q_2}+1)(n^0_{q_3}+1) L^{q_2,q_3}_{q_1} \} \qquad (13)$$

For phonon scattered by other sources, we can use a relaxation time approximation by writing:

$$\left(\frac{\partial n_{q_1}}{\partial t}\right)_{other} = -\frac{dn_{q_1}}{\tau_{q_1}} = -\beta \frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}} \Phi_{q_1} \qquad (14)$$

Now, let's write Φ_q linear in ∇T:

$$\Phi_q = \sum_i f_{q,i} \, (\nabla T)_i \qquad (15)$$

where i denote cartesian direction. Equation.2 can be written in terms of $f_{q,i}$:

$$-\frac{1}{\beta} v_{q_1,i} \frac{\partial n^0_{q_1}}{\partial T} = \sum_{q_2,q_3} \{ \ (f_{q_1,i} + f_{q_2,i} - f_{q_3,i})\, n^0_{q_1} n^0_{q_2} (n^0_{q_3}+1) L^{q_3}_{q_1,q_2} \qquad (16)$$

$$+\frac{1}{2} (f_{q_1,i} - f_{q_2,i} - f_{q_3,i})\, n^0_{q_1} (n^0_{q_2}+1)(n^0_{q_3}+1) L^{q_2,q_3}_{q_1} \} + \frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}} f_{q_1,i} \qquad (17)$$

Writing out explicitly the transition probability $L^{q_3}_{q_1,q_2}$ and $L^{q_1}_{q_2,q_3}$, we have:

$$L^{q_3}_{q_1,q_2} = \frac{2\pi}{\hbar} |V^{(3)}(q_1, q_2, -q_3)|^2 \delta(\omega_1 + \omega_2 - \omega_3) \qquad (18)$$

$$L^{q_2,q_3}_{q_1} = \frac{2\pi}{\hbar} |V^{(3)}(q_1, -q_2, -q_3)|^2 \delta(\omega_1 - \omega_2 - \omega_3) \qquad (19)$$

with the interaction $V^{(3)}(q_1, q_2, q_3)$ as:

$$V^{(3)}(q_1,q_2,q_3) = \left(\frac{\hbar}{2N}\right)^{\frac{3}{2}} \sum_{\kappa_1,\kappa_2,\kappa_3} \sum_{R_1,R_2,R_3} \sum_{\alpha,\beta,\gamma} \frac{\varepsilon^{\kappa_1}_{\alpha}(q_1)\varepsilon^{\kappa_2}_{\beta}(q_2)\varepsilon^{\kappa_3}_{\gamma}(q_3)}{\sqrt{\omega_1\omega_2\omega_3}\sqrt{M_{\kappa_1}M_{\kappa_2}M_{\kappa_3}}}$$

$$exp\left[i(q_1R_1 + q_2R_2 + q_3R_3)\right] \Phi^{\kappa_1,\kappa_2,\kappa_3}_{\alpha,\beta,\gamma}(R_1,R_2,R_3) \qquad (20)$$

which is non-zero only when $k1 + k2 + k3 = 0$. the transport equation Eq.17 is then becomes:

$$-\frac{1}{\beta} v_{q_1,i} \frac{\partial n^0_{q_1}}{\partial T} = \sum_{q_2,q_3} \{ \ (f_{q_1,i} + f_{q_2,i} - f_{q_3,i})\, n^0_{q_1} n^0_{q_2} (n^0_{q_3}+1) L^{q_3}_{q_1,q_2}$$

$$+\frac{1}{2} (f_{q_1,i} - f_{q_2,i} - f_{q_3,i})\, n^0_{q_1} (n^0_{q_2}+1)(n^0_{q_3}+1) L^{q_2,q_3}_{q_1} \} + \frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}} f_{q_1,i} \qquad (21)$$

now, writing out explicitly the term $L^{q_3}_{q_1,q_2}$ and $L^{q_2,q_3}_{q_1}$ in Eq.21 with δ functions for energy and crystal momentum conservation and ignore the final term, we have:

$$
\begin{aligned}
&-\frac{1}{\beta}v_{q_1,i}\frac{\partial n^0_{q_1}}{\partial T} = \\
&\frac{2\pi}{\hbar}\sum_{q_2,q_3}\{\ (f_{q_1,i}+f_{q_2,i}-f_{q_3,i})\, n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)|V^{(3)}(q_1,q_2,-q_3)|^2\delta(\omega_1+\omega_2-\omega_3)\delta(q_1+q_2-q_3)\} \\
+&\frac{1}{2}\frac{2\pi}{\hbar}\sum_{q_2,q_3}\{\ (f_{q_1,i}-f_{q_2,i}-f_{q_3,i})\, n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(\omega_1-\omega_2-\omega_3)\delta(q_1-q_2-q_3)\} \\
=&\frac{2\pi}{\hbar}\sum_{q_2,q_3}\{\ (f_{q_1,i}+f_{-q_2,i}-f_{q_3,i})\, n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(\omega_1+\omega_2-\omega_3)\delta(q_1-q_2-q_3)\} \\
+&\frac{1}{2}\frac{2\pi}{\hbar}\sum_{q_2,q_3}\{\ (f_{q_1,i}-f_{q_2,i}-f_{q_3,i})\, n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(\omega_1-\omega_2-\omega_3)\delta(q_1-q_2-q_3)\}
\end{aligned} \tag{22}
$$

where we have changed the dummy summation index from $-q_2 \rightarrow q_2$ and use the fact that $n^0_{q_2} = n^0_{-q_2}$; $\omega_{q_2} = \omega_{-q_2}$. So Eq.21 can be simpled to:

$$
\begin{aligned}
-\frac{1}{\beta}v_{q_1,i}\frac{\partial n^0_{q_1}}{\partial T} = \frac{2\pi}{\hbar}\sum_{q_2,q_3}&|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(q_1-q_2-q_3) \\
&\{\ (f_{q_1,i}+f_{-q_2,i}-f_{q_3,i})\, n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3) \\
&+\frac{1}{2}(f_{q_1,i}-f_{q_2,i}-f_{q_3,i})\, n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)\}
\end{aligned} \tag{23}
$$

We define Q and W_i to be:

$$
\begin{aligned}
Q_1 = \frac{2\pi}{\hbar}\sum_{q_2,q_3}&|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(q_1-q_2-q_3) \\
&\{\ n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3)+\frac{1}{2}n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)\}
\end{aligned} \tag{24}
$$

$$
\begin{aligned}
W^n_{1,i} = \frac{2\pi}{\hbar}\sum_{q_2,q_3}&|V^{(3)}(q_1,-q_2,-q_3)|^2\delta(q_1-q_2-q_3) \\
&\{\ (f_{-q_2,i}-f_{q_3,i})\, n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3) \\
&\quad -\frac{1}{2}(f_{q_2,i}+f_{q_3,i})\, n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)\}
\end{aligned} \tag{25}
$$

so that Eq.21 becomes:

$$
-\frac{1}{\beta}v_{q_1,i}\frac{\partial n^0_{q_1}}{\partial T} = \left(Q_1+\frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}}\right)f_{q_1,i}+W_{1,i} = Q'_1 f_{q_1,i}+W_{1,i} \tag{26}
$$

Iteration starts with:

$$
f^0_{q_1,i} = \frac{-v_{q_1,i}\frac{\partial n^0_{q_1}}{\partial T}}{\beta Q'_1} \tag{27}
$$

and is updated by:

$$
f^{(n+1)}_{q_1,i} = -(\frac{1}{\beta}v_{q_1,i}\frac{\partial n^0_{q_1}}{\partial T}+W^n_{1,i})/Q'_1 \tag{28}
$$

3 Thermal conductivity

The lattice thermal conductivity is given by:

$$
J_{phonon,i} = \frac{1}{N_k\Omega}\sum_q \hbar\omega_q v_{q,i} dn_{q,j} = -\sum_j \kappa_{i,j}\left(\nabla T\right)_j \tag{29}
$$

where $dn_q = \sum_i \beta n_q^0 (n_q^0 + 1) f_{q,i} \left(\nabla T\right)_i$. We then find the thermal conductivity to be:

$$\kappa_{i,j} = -\frac{1}{N_k \Omega} \sum_q \hbar \omega_q v_{q,i} \beta n_q^0 (n_q^0 + 1) f_{q,j} \tag{30}$$

4 Direct solution of phonon transport equation

The direct solution of phonon BTE can be obtained by writing in matrix form. Starting from Eq.17, we can write:

$$\sum_{q_2} A_{q_1,q_2} f_{q_2,i} = b_{q_1,i} \tag{31}$$

where i indicate cartesian direction, the terms are defined by:

$$b_{q_1,i} = -\frac{1}{\beta} v_{q_1,i} \frac{\partial n^0_{q_1}}{\partial T} = -\hbar\omega_1 v_{q_1,i} n^0_{q_1}(n^0_{q_1}+1)\frac{1}{T} \tag{32}$$

$$\Lambda^{q_3}_{q_1,q_2} = n^0_{q_1} n^0_{q_2}(n^0_{q_3}+1) L^{q_3}_{q_1,q_2} \tag{33}$$

$$\Lambda^{q_2,q_3}_{q_1} = n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1) L^{q_2,q_3}_{q_1} \tag{34}$$

$$\tag{35}$$

and the matrix:

$$A_{q_1,q_2} = \frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau}\delta_{q_1,q_2} - \sum_{q_3}\left(\Lambda^{q_2}_{q_1,q_3} - \Lambda^{q_2}_{q_1,q_2} + \Lambda^{q_2,q_3}_{q_1}\right) \tag{36}$$

where τ is defined to be:

$$\frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}} = \sum_{q_3,q_4}\left\{\Lambda^{q_4}_{q_1,q_3} + \frac{1}{2}\Lambda^{q_3,q_4}_{q_1}\right\} + \frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau_{q_1}} \tag{37}$$

To see the origin of the second term in Eq.36, ew can write:

$$\begin{aligned}
&\sum_{q_2,q_3}\left\{(f_{q_2,i} - f_{q_3,i})\Lambda^{q_3}_{q_1,q_2} - \frac{1}{2}(f_{q_2,i} + f_{q_3,i})\Lambda^{q_2,q_3}_{q_1}\right\} \\
&= \sum_{q_2,q_3}(\Lambda^{q_3}_{q_1,q_2} - \frac{1}{2}\Lambda^{q_2,q_3}_{q_1}) f_{q_2,i} - \sum_{q_2,q_3}(\Lambda^{q_3}_{q_1,q_2} + \frac{1}{2}\Lambda^{q_2,q_3}_{q_1}) f_{q_3,i} \\
&= \sum_{q_2,q_3}(\Lambda^{q_3}_{q_1,q_2} - \frac{1}{2}\Lambda^{q_2,q_3}_{q_1}) f_{q_2,i} - \sum_{q_2,q_3}(\Lambda^{q_2}_{q_1,q_3} + \frac{1}{2}\Lambda^{q_3,q_2}_{q_1}) f_{q_2,i} \\
&= \sum_{q_2,q_3}\left(\Lambda^{q_3}_{q_1,q_2} - \Lambda^{q_2}_{q_1,q_3} - \Lambda^{q_2,q_3}_{q_1}\right) f_{q_2,i} \\
&= -\sum_{q_2,q_3}\left(\Lambda^{q_2,q_3}_{q_1} - \Lambda^{q_3}_{q_1,q_2} + \Lambda^{q_2}_{q_1,q_3}\right) f_{q_2,i}
\end{aligned} \tag{38}$$

Eq.31 ($AF_i = b_i$) can be solved by:

$$F_i = A^+ b_i + (I - A^+A)y \tag{39}$$

with A^+ the pseudoinverse of A and $(I - A^+A)y$ with arbitrary y arise when the solution is not unique.

The direct solution can be simplified further. First, we define

$$\begin{aligned}
A^{in}_{q_1,q_2} &= -\sum_{q_3}\left(\Lambda^{q_2}_{q_1,q_3} - \Lambda^{q_2}_{q_1,q_2} + \Lambda^{q_2,q_3}_{q_1}\right) \\
&= -\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,q_3)|^2 n^0_{q_1} n^0_{q_3}(n^0_{q_2}+1)\delta(\omega_1+\omega_3-\omega_2) \\
&\quad + \frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,q_2,-q_3)|^2 n^0_{q_1} n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3) \\
&\quad - \frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,-q_3)|^2 n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)
\end{aligned} \tag{40}$$

The second term can be modified by changing the summation index q_3 into $q_3' = -q_3$ as:

$$
\begin{aligned}
&-\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,q_2,-q_3)|^2 n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3) \\
=&\frac{2\pi}{\hbar}\sum_{q_3'=-q_3}|V^{(3)}(q_1,q_2,q_3')|^2 n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3) \\
=&\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,q_2,q_3)|^2 n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3)
\end{aligned}
\tag{41}
$$

we do the same for the third term:

$$
\begin{aligned}
&-\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,-q_3)|^2 n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3) \\
=&\frac{2\pi}{\hbar}\sum_{q_3'=-q_3}|V^{(3)}(q_1,-q_2,q_3')|^2 n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3) \\
=&\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,q_3)|^2 n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)
\end{aligned}
\tag{42}
$$

so that

$$
\begin{aligned}
A^{in}_{q_1,q_2} =& -\sum_{q_3}\left(\Lambda^{q_2}_{q_1,q_3}-\Lambda^{q_2}_{q_1,q_2}+\Lambda^{q_2,q_3}_{q_1}\right) \\
=& -\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,q_3)|^2\left[n^0_{q_1}n^0_{q_3}(n^0_{q_2}+1)\delta(\omega_1+\omega_3-\omega_2)+n^0_{q_1}(n^0_{q_2}+1)(n^0_{q_3}+1)\delta(\omega_1-\omega_2-\omega_3)\right] \\
&+\frac{2\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,q_2,q_3)|^2 n^0_{q_1}n^0_{q_2}(n^0_{q_3}+1)\delta(\omega_1+\omega_2-\omega_3)
\end{aligned}
\tag{43}
$$

define short hands for the above equations:

$$
A^{in}_{q_1,q_2} = I_{q_1,q_2}(-B_{q_1,q_2}+C_{q_1,q_2}) \tag{44}
$$

$$
B_{q_1,q_2} = \frac{\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,-q_2,q_3)|^2\frac{1}{sinh(\beta\hbar\omega_3/2)}\left\{\delta(\omega_1+\omega_3-\omega_2)+\delta(\omega_1-\omega_2-\omega_3)\right\} \tag{45}
$$

$$
C_{q_1,q_2} = \frac{\pi}{\hbar}\sum_{q_3}|V^{(3)}(q_1,q_2,q_3)|^2\frac{1}{sinh(\beta\hbar\omega_3/2)}\delta(\omega_1+\omega_2-\omega_3) \tag{46}
$$

$$
I_{q_1,q_2} = \sqrt{n_{q_1^0}(n^0_{q_1}+1)n^0_{q_2}(n^0_{q_2}+1)} \tag{47}
$$

Eq.31 can now be written as:

$$
\begin{aligned}
b_{q_1,i} =& \sum_{q_2}\left(\frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau}\delta_{q_1,q_2}-I_{q_1,q_2}B_{q_1,q_2}+I_{q_1,q_2}C_{q_1,q_2}\right)f_{q_2,i} \\
=& \sum_{q_2}\left(\frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau}\delta_{q_1,q_2}+I_{q_1,q_2}C_{q_1,q_2}\right)f_{q_2,i}-\sum_{q_2}I_{q_1,q_2}B_{q_1,q_2}f_{q_2,i}
\end{aligned}
\tag{48}
$$

since $f_{q_2,i} = -f_{-q_2,i}$, we have:

$$
\begin{aligned}
&-\sum_{q_2'}I_{q_1,q_2'}B_{q_1,q_2'}f_{q_2',i} \\
&= -\sum_{q_2=-q_2'}I_{q_1,q_2'}B_{q_1,q_2'}f_{q_2',i} \\
&= -\sum_{q_2}I_{q_1,-q_2}B_{q_1,-q_2}f_{-q_2,i} \\
&= \sum_{q_2}I_{q_1,q_2}B_{q_1,-q_2}f_{q_2,i}
\end{aligned}
\tag{49}
$$

So that

$$b_{q_1,i} = \sum_{q_2} \left(\frac{n^0_{q_1}(n^0_{q_1}+1)}{\tau} \delta_{q_1,q_2} + I_{q_1,q_2}(B_{q_1,-q_2} + C_{q_1,q_2}) \right) f_{q_2,i}$$

and the term $B_{q_1,-q_2} + C_{q_1,q_2}$ can be written as:

$$B_{q_1,-q_2} + C_{q_1,q_2} = \frac{\pi}{\hbar} \sum_{q_3} |V^{(3)}(q_1,q_2,q_3)|^2 \frac{1}{sinh(\beta\hbar\omega_3/2)} \\ \{\delta(\omega_1+\omega_3-\omega_2) + \delta(\omega_1-\omega_2-\omega_3) + \delta(\omega_1+\omega_2-\omega_3)\} \tag{50}$$

now we can see that only a single matrix element need to be computed for each q_1, q_2, q_3 triplet.

5 Solving the Irreducible Brillouin zone

Using k to refer to a point in the irreducible Brillouin zone and q to a general point in reciprocal space, we can write Eq.31 to be:

$$b_{k_1,i} = \sum_{q_2} A_{k_1,q_2} f_{q_2,i} \tag{51}$$

$$= \sum_{k_2} \sum_{R} A_{k_1,Rk_2} f_{Rk_2,i} \tag{52}$$

where the sum is over symmetry operations R that generate a general q_2 from k_2 in the irBZ. for $f_{Rk_2,i}$, it transform under rotation:

$$f_{Rk_2,i} = \sum_j R_{ij} f_{k_2,j} \tag{53}$$

so now we can write Eq.52 as:

$$b_{k_1,i} = \sum_{k_2} \sum_{j} \left(\sum_{R} R_{ij} A_{k_1,Rk_2} \right) f_{k_2,j} \\ = \sum_{k_2} \sum_{j} \Omega_{i,k_1,j,k_2} f_{k_2,j} \tag{54}$$

now the matrix Ω will have the dimension $3 \times n_s \times n_{k,ir}$.