Boltzmann Transport Equation

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1 Boltzmann Equation

The general Boltzmann transport equation (BTE) is given as

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f + \frac{1}{\hbar} \mathbf{F}_{ext} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{coll}. \tag{1}$$

The bulk-bulk scattering collision integral is given as

$$\left(\frac{\partial f}{\partial t} \right)_{coll} = \mathcal{I}^{(bb)}_{\mathbf{k}} = \int \frac{d\mathbf{k'}}{(2\pi)^3} \{ W^{(bb)}_{\mathbf{k},\mathbf{k'}} f_{\mathbf{k'}} (1 - f_{\mathbf{k}}) - W^{(bb)}_{\mathbf{k'},\mathbf{k}} f_{\mathbf{k}} (1 - f_{\mathbf{k'}}) \} \tag{2}$$

where $W^{(bb)}_{\mathbf{k},\mathbf{k'}}$ is the bulk-bulk transition rate which we calculate according to Fermi's Golden rule. $f(\mathbf{r}, \mathbf{k}, t)$ is the distribution function, i.e., the probability that state (wavepacket- made superposition of Bloch eigenstates; semiclassically) $\mathbf{k}$ is occupied at time t near $\mathbf{r}$; under no external fields it is the Fermi-Dirac distribution ($f(\mathbf{r}, \mathbf{k}, t) = f^0_{\mathbf{k}}$). Below we solve the BTE by linearizing it and finding conductivity tensor formula.

2 Linearized BTE: Finding conductivity tensor

The Boltzmann equation under only external electric field (weak and constant) $\mathbf{E}$ becomes

$$-e\mathbf{E} \cdot \partial_{\mathbf{k}} f_{\mathbf{k}} = \mathcal{I}^{(bb)}_{\mathbf{k}}. \tag{3}$$

In the quasi-elastic approximation with linearized distribution function ($f_{\mathbf{k}} = f^0_{\mathbf{k}} - \varphi_{\mathbf{k}} \frac{\partial f^0_{\mathbf{k}}(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}}$) the BTE becomes

$$e \frac{\partial f^0_{\mathbf{k}}}{\partial \varepsilon_{\mathbf{k}}} \big[\mathbf{E} \cdot \mathbf{v}(\mathbf{k}) \big] = \left(\frac{\partial f}{\partial t} \right)_{coll} \tag{4}$$

$$\implies -e\mathbf{E} \cdot \mathbf{v}(\mathbf{k}) = \mathcal{J}^{(bb)}_{\mathbf{k}}. \tag{5}$$

where $\mathcal{J}_{\mathbf{k}}^{(bb)}$ is given as

$$\mathcal{J}_{\mathbf{k}}^{(bb)} = \int \frac{d\mathbf{k'}}{(2\pi)^3} \mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)} (\varphi_{\mathbf{k'}}^{(b)} - \varphi_{\mathbf{k}}^{(b)}) \tag{6}$$

and the $\mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)}$ is obtained for different problems differently. For example it takes the form of Eqn. (20) for e-ph scattering. Incase of a elastic impurity scattering, we use $W_{\mathbf{k},\mathbf{k'}}^{(bb)} = W_{\mathbf{k'},\mathbf{k}}^{(bb)}$, which simplifies the collision integral written in lowest order of $\varphi_{\mathbf{k}}$ as

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \int \frac{d\mathbf{k'}}{(2\pi)^3} W_{\mathbf{k},\mathbf{k'}}^{(bb)} (f_{\mathbf{k'}} - f_{\mathbf{k}}) = -\int \frac{d\mathbf{k'}}{(2\pi)^3} \frac{\partial f^0}{\partial \varepsilon} W_{\mathbf{k},\mathbf{k'}}^{(bb)} (f_{\mathbf{k'}} - f_{\mathbf{k}}) \tag{7}$$

implying $\mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)} = W_{\mathbf{k},\mathbf{k'}}^{(bb)}$. Taking the ansatz

$$\varphi_{\mathbf{k}}^{(b)} = (\mathbf{E} \cdot \hat{k}) \Lambda(\varepsilon_{\mathbf{k}}) \tag{8}$$

$$\implies -e\mathbf{E} \cdot \mathbf{v}(\mathbf{k}) = \int \frac{d\mathbf{k'}}{(2\pi)^3} \mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)} (\varphi_{\mathbf{k'}}^{(b)} - \varphi_{\mathbf{k}}^{(b)}) \tag{9}$$

$$e\mathbf{E} \cdot \mathbf{v}(\mathbf{k}) = \Lambda(\varepsilon_{\mathbf{k}}) \mathbf{E} \cdot [\int \frac{d\mathbf{k'}}{(2\pi)^3} \mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)} (\hat{k} - \hat{k}')] \tag{10}$$

If scattering is azimuthally symmetric around $\mathbf{k}$, then

$$\begin{aligned} e\mathbf{E} \cdot \mathbf{v}(\mathbf{k}) &= \Lambda(\varepsilon_{\mathbf{k}}) (\mathbf{E} \cdot \hat{k}) \underbrace{\int \frac{d\mathbf{k'}}{(2\pi)^3} \mathcal{W}_{\mathbf{k'},\mathbf{k}}^{(bb)} (1 - \hat{k}' \cdot \hat{k})}_{1/\tau(\mathbf{k})} \\ &= \frac{\Lambda(\varepsilon_{\mathbf{k}})(\mathbf{E} \cdot \hat{k})}{\tau(\mathbf{k})} = \frac{\varphi_{\mathbf{k}}^{(b)}}{\tau(\mathbf{k})} \\ \implies \varphi_{\mathbf{k}}^{(b)} &= e(\mathbf{E} \cdot \mathbf{v}(\mathbf{k})) \tau(\mathbf{k}) \end{aligned} \tag{11}$$

The current density is given as

$$\mathbf{J} = 2e \int \frac{d\mathbf{k}}{(2\pi)^3} \mathbf{v}(\mathbf{k}) f_{\mathbf{k}} = -2e \int \frac{d\mathbf{k}}{(2\pi)^3} \mathbf{v}(\mathbf{k}) \varphi_{\mathbf{k}}^{(b)} \frac{\partial f_{\mathbf{k}}^0(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}} \tag{12}$$

Substituting the value of $\varphi_{\mathbf{k}}^{(b)}$, we get

$$\mathbf{J} = -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} \mathbf{v}(\mathbf{k}) (\mathbf{E} \cdot \mathbf{v}(\mathbf{k})) \tau(\mathbf{k}) \frac{\partial f_{\mathbf{k}}^0(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}}. \tag{13}$$

Using the Ohm's law

$$\begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}, \tag{14}$$

we get

$$\sigma_{ij} = -2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} v_i(\mathbf{k}) v_j(\mathbf{k}) \tau(\mathbf{k}) \frac{\partial f^0_{\mathbf{k}}(\varepsilon_{\mathbf{k}})}{\partial \varepsilon_{\mathbf{k}}} \tag{15}$$

The negative gradient of the distribution function acts as a delta function (as $k_B T \ll \mu$) at low temperatures

$$\sigma_{ij} = 2e^2 \int \frac{d\mathbf{k}}{(2\pi)^3} v_i(\mathbf{k}) v_j(\mathbf{k}) \tau(\mathbf{k}) \delta(\varepsilon_{\mathbf{k}} - \mu) \tag{16}$$

The **transport lifetime** τ_{tr} is given as

$$\frac{1}{\tau_{tr}} = \frac{1}{\tau(\varepsilon_{\mathbf{k}} = \mu)} = \int \frac{d\mathbf{k}'}{(2\pi)^3} \mathcal{W}^{(bb)}_{\mathbf{k}',\mathbf{k}} (1 - \hat{k}' \cdot \hat{k}) \tag{17}$$

2.1 Electron-Phonon scattering

The transition rate for electron-phonon scattering problem can be found by taking the phonons to be in thermal equilibrium at temperature T. The expression for $W^{(bb)}_{\mathbf{k},\mathbf{k}'}$ can be written as

$$W^{(bb)}_{\mathbf{k},\mathbf{k}'} = 2\pi |\mathcal{G}^{(bbl)}_{\mathbf{k},\mathbf{k}'}|^2 \left\{ n_B(\Omega^{(l)}_{\mathbf{q}}) \delta(\varepsilon^{(b)}_{\mathbf{k}'} - \varepsilon^{(b)}_{\mathbf{k}} - \Omega^{(l)}_{\mathbf{q}}) + [n_B(\Omega^{(l)}_{\mathbf{q}}) + 1] \delta(\varepsilon^{(b)}_{\mathbf{k}'} - \varepsilon^{(b)}_{\mathbf{k}} + \Omega^{(l)}_{\mathbf{q}}) \right\}, \tag{18}$$

with $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ and the bulk-bulk amplitudes $\mathcal{G}^{(bbl)}_{\mathbf{k},\mathbf{k}'}$ given as

$$\mathcal{G}^{(bbl)}_{\mathbf{k},\mathbf{k}'} = i \frac{g_0 \sqrt{\Omega^{(l)}_{\mathbf{q}}}}{c_l \sqrt{2\rho_M}} \langle u_{\mathbf{k}'} | u_{\mathbf{k}} \rangle. \tag{19}$$

Here $n_B(\Omega)$ is the Bose-Einstein function with zero chemical potential.

$$\mathcal{W}^{(bb)}_{\mathbf{k}',\mathbf{k}} = 2\pi |\mathcal{G}^{(bbl)}_{\mathbf{k}',\mathbf{k}}|^2 \left\{ [n_B(\Omega^{(l)}_{\mathbf{q}}) + n_F(\varepsilon^{(b)}_{\mathbf{k}} + \Omega^{(l)}_{\mathbf{q}})] \delta(\varepsilon^{(b)}_{\mathbf{k}'} - \varepsilon^{(b)}_{\mathbf{k}} - \Omega^{(l)}_{\mathbf{q}}) + [n_B(\Omega^{(l)}_{\mathbf{q}}) + 1 - n_F(\varepsilon^{(b)}_{\mathbf{k}} - \Omega^{(l)}_{\mathbf{q}})] \delta(\varepsilon^{(b)}_{\mathbf{k}'} - \varepsilon^{(b)}_{\mathbf{k}} + \Omega^{(l)}_{\mathbf{q}}) \right. \tag{20}$$