Solution by orthogonal polynomial expansion

- Another useful technique for solving the BTE is by expanding the solution in a set of orthogonal polynomials, such as Legendre polynomials $P_m(\cos\theta)$. The rationale behind this is that the electric field breaks the symmetry of the system and introduces a prefered axis along which a shift of the distribution occurs. Since there is no breaking of the symmetry in the asimuthal plane, we have a system with cylindrical symmetry. (When the electric field varies in two dimensions, Legendre polynomials will be replaced by spherical harmonics).

- Therefore, in cases where we have cylindrical symmetry, where the electric field is aligned with the polar axis, the distribution function can be expanded as:

$$f(z,\vec{k},t) = \sum_{l=0}^{\infty} \underbrace{f_l(z,k,t)}_{\text{Weighting coefficient}} \underbrace{P_l(\cos\theta)}_{\text{Legendre polynomial}}$$

The Legendre polynomials are defined as:

$$P_0 = 1,\ P_1 = \cos\theta,\ P_2 = \frac{3}{2}\cos^2\theta - \frac{1}{2}$$

and the orthogonality relation is

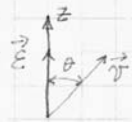
$$\int_{-1}^{1} P_l P_m \, d(\cos\theta) = \frac{2}{2l+1}\delta_{lm}$$

- For isotropic and elastic scattering one needs to keep terms up to $l=1$. This is essentially the basis for the RTA. If the scattering is not predominantly elastic or isotropic, higher-order terms need to be kept in the series. For example, for polar optical phonon scattering, almost all of the terms are needed to describe high field transport, which makes the method rather useles.

- Note also that by using this method, in some special cases, one can obtain both low-field and high-field properties of the system.

- To illustrate the method, let us consider the case when the electric field is along the z-axis and there are no spatial gradients. Furthermore, if we are interested only in the steady-state solution, the Boltzmann Transport equation becomes:

$$-\frac{e}{\hbar}\vec{\mathcal{E}}\cdot\nabla_k f = \left.\frac{\partial f}{\partial t}\right|_{coll}$$



Taking only two terms of the expansion for f, i.e.

$$f = f_0 + f_1\cos\theta = f_0 + k g_1\cos\theta = f_0 + k_z g_1(E)$$

↖ This is <u>not</u> the equilibrium D.F.

leads to the following expression on the LHS:

$$-\frac{e}{\hbar}\vec{\mathcal{E}}\cdot\hbar\vec{v}\frac{\partial f}{\partial E} = -\frac{e}{\hbar}\mathcal{E}_z\frac{\partial f}{\partial k_z} = -\frac{e}{\hbar}\mathcal{E}_z\frac{\partial}{\partial k_z}\left(f_0 + k_z g_1(E)\right]$$

$$= -\frac{e}{\hbar}\mathcal{E}_z\left[\frac{\partial f_0}{\partial k_z} + g_1(E) + k_z\frac{\partial g_1}{\partial k_z}\right]$$

We can further simplify the LHS by using: $E = \frac{\hbar^2 k_z^2}{2m^*} + E_{xy} \Rightarrow \frac{\partial E}{\partial k_z} = \frac{\hbar^2 k_z}{m^*}$

$$LHS = -\frac{e}{\hbar}\mathcal{E}_z\left[\frac{\partial f_0}{\partial E}\frac{\partial E}{\partial k_z} + g_1(E) + k_z\frac{\partial g_1}{\partial E}\frac{\partial E}{\partial k_z}\right]$$

$$= -\frac{e}{\hbar}\mathcal{E}_z\left[\hbar v_z\frac{\partial f_0}{\partial E} + g_1(E) + \hbar k_z v_z\frac{\partial g_1}{\partial E}\right]$$

$$= -\frac{e\mathcal{E}_z}{\hbar}\left[\hbar v\frac{\partial f_0}{\partial E}\cos\theta + g_1(E) + m^* v^2\frac{\partial g_1}{\partial E}\cos^2\theta\right]$$

When this result is substituted back in the BTE, we get:

$$-\frac{e\mathcal{E}_z}{\hbar}\left[\hbar v\frac{\partial f_0}{\partial E}\underbrace{\cos\theta}_{P_1} + \underset{P_0}{g_1(E)} + m^* v^2\frac{\partial g_1}{\partial E}\underbrace{\cos^2\theta}_{P_2?}\right] = \underset{P_0}{\left.\frac{\partial f_0}{\partial t}\right|_{coll}} + \underset{P_1}{k\cos\theta\left.\frac{\partial g_1}{\partial t}\right|_{coll.}}$$

- If one integrates against $d(\cos\theta)$ this last result, it would find that:

$$-\frac{e\mathcal{E}_z}{\hbar}\left[\cancel{2}\,g_1(E) + \underbrace{m^* v^2}_{2E}\,\frac{\partial g_1}{\partial E}\,\frac{\cancel{2}}{3}\right] = \cancel{2}\,\frac{\partial f_0}{\partial t}\Big|_{coll}$$

or:

$$\boxed{-\frac{e\mathcal{E}_z}{\hbar}\left[g_1(E) + \frac{2}{3}E\,\frac{\partial g_1}{\partial E}\right] = \frac{\partial f_0}{\partial t}\Big|_{coll}} \quad (1)$$

- First multiplying by $\cos\theta$ and integrating against $d(\cos\theta)$ gives:

$$-\frac{e\mathcal{E}_z}{\cancel{\hbar}}\,\cancel{\hbar v}\,\frac{\cancel{2}}{3}\,\frac{\partial f_0}{\partial E} = k\,\frac{\partial g_1}{\partial t}\Big|_{coll}\,\frac{\cancel{2}}{\cancel{3}}$$

$$k = \frac{m^* v}{\hbar}$$

$$\boxed{-e\mathcal{E}_z\,\frac{\partial f_0}{\partial E} = \frac{m^*}{\hbar}\,\frac{\partial g_1}{\partial t}\Big|_{coll}} \quad (2)$$

- → The <u>inelastic</u> part of the e-phonon interaction provides relaxation of the <u>$l=0$ component</u> (the isotropic part of the distribution),
  → The <u>elastic</u> part of the e-phonon interaction provides relaxation of the <u>$l=1$ component</u> of the distribution, for which the RTA approximation is applicable; i.e. $\partial g_1/\partial t|_{coll} = -\frac{g_1}{\tau_m}$. This, when substituted back into equation (2), gives:

$$-e\mathcal{E}_z\,\frac{\partial f_0}{\partial E} = -\frac{m^*}{\hbar}\,\frac{g_1}{\tau_m} \quad \Rightarrow \quad g_1(E) = +e\mathcal{E}_z\,\frac{\hbar}{m^*}\,\frac{\partial f_0}{\partial E}\,\tau_m(E)$$

Hence:

$$\boxed{g_1(E) = e\mathcal{E}_z\,\frac{\hbar}{m^*}\,\tau_m(E)\,\frac{\partial f_0}{\partial E}} \quad (3)$$

- For acoustic deformation potential scattering, we have:

$$\tau_m(E) = \frac{\pi\hbar^4\rho v_s^2}{m^*\Xi_{ac}^2 k_B T}\,\frac{1}{\sqrt{2m^* E_k}}$$

If we introduce the mean free path L between scattering events as:

$$L = v\,\tau_m(E) = \sqrt{\frac{2E_K}{m^*}}\;\frac{\pi\hbar^4\rho v_s^2}{m^{*3/2}\Xi_{ac}^2 k_BT}\;\frac{1}{\sqrt{2E_K}} = \frac{\pi\hbar^4\rho v_s^2}{m^{*2}\Xi_{ac}^2 k_BT}$$

which does not depend upon the carrier energy, we have:

$$\tau_m(E) = \frac{L}{v} = \sqrt{\frac{m^*}{2E_K}}\;\frac{\pi\hbar^4\rho v_s^2}{m^{*2}\Xi_{ac}^2 k_BT} = \sqrt{\frac{m^*}{2E_K}}\,L$$

Substituting this back into our expression for $g_1(E)$ finally gives:

$$g_1(E) = e\mathcal{E}_z\frac{\hbar}{m^*}\,L\sqrt{\frac{m^*}{2E_K}}\;\frac{\partial f_0}{\partial E} = \boxed{\frac{\hbar e\mathcal{E}_z L}{\sqrt{2m^*E_K}}\;\frac{\partial f_0}{\partial E} = g_1(E)} \quad (4)$$

- When this result is inserted into the $l=0$ component of the BTE involving the angular independend distribution f_0, one gets:

$$-\frac{e\mathcal{E}_z}{\hbar}\left[\frac{\hbar e\mathcal{E}_z L}{\sqrt{2m^*}}\,E_K^{-1/2}\frac{\partial f_0}{\partial E} + \frac{2}{3}E\,\frac{\hbar e\mathcal{E}_z L}{\sqrt{2m^*}}\,\frac{\partial}{\partial E}\left(E^{-1/2}\frac{\partial f_0}{\partial E}\right)\right] = \frac{\partial f_0}{\partial t}\bigg|_{coll}$$

or:

$$-\frac{e\mathcal{E}_z}{\hbar}\,\frac{\hbar e\mathcal{E}_z L}{\sqrt{2m^*}}\underbrace{\left[E_K^{-1/2}\frac{\partial f_0}{\partial E} + \frac{2}{3}E\left(-\frac{1}{2}E^{-3/2}\frac{\partial f_0}{\partial E} + E^{-1/2}\frac{\partial^2 f_0}{\partial E^2}\right)\right]} = \frac{\partial f_0}{\partial t}\bigg|_{coll}$$

$$E_K^{-1/2}\frac{\partial f_0}{\partial E} - \frac{1}{3}E_K^{-1/2}\frac{\partial f_0}{\partial E} + \frac{2}{3}E^{1/2}\frac{\partial^2 f_0}{\partial E^2} =$$

$$= \frac{2}{3}E_K^{-1/2}\frac{\partial f_0}{\partial E} + \frac{2}{3}E_K^{1/2}\frac{\partial^2 f_0}{\partial E^2} = \frac{2}{3}E_K^{-1/2}\left(\frac{\partial f_0}{\partial E} + E\frac{\partial^2 f_0}{\partial E^2}\right)$$

To summarize:

$$\boxed{-\frac{(e\mathcal{E}_z)^2 L}{\sqrt{2m^*E_K}}\;\frac{2}{3}\left(\frac{\partial f_0}{\partial E} + E\frac{\partial^2 f_0}{\partial E^2}\right) = \frac{\partial f_0}{\partial t}\bigg|_{coll.}} \quad (5)$$

- The next task in this analysis is to calculate the collision operator on the RHS for acoustic deformation potential scattering, for the general case of inelastic scattering process. It will be assumed that the phonons are in equilibrium, i.e. equilibrium distribution function will be used in the calculation of the occupancy.

Therefore; for non-degenerate semiconductors, one has:

$$\left.\frac{\partial f_0}{\partial t}\right|_{coll.} = \sum_{\vec{k}'}\left[f_0(\vec{k}')\,S(\vec{k}',\vec{k}) - S(\vec{k},\vec{k}')f_0(\vec{k})\right]$$

where the transition rates $S(\vec{k},\vec{k}')$ and $S(\vec{k}',\vec{k})$ are of the form:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\frac{\hbar\Xi_{ac}^2 q^2}{2\rho V\omega_q}\left(N_q + \frac{1}{2} \overset{\text{abs.}}{\underset{\text{em.}}{\mp}} \frac{1}{2}\right)\underbrace{\delta(E_{k'} - E_k \mp \hbar\omega_q)\,\delta(\vec{k} \pm \vec{q} - \vec{k}')}$$

when combined into a single δ-function these two terms will yield a factor $\frac{m^*}{\hbar^2 kq}$ and limits on the wavevector q: $\quad 0 \le q \le 2k\left(1 \pm \frac{v_s}{v}\right)$

$$S(\vec{k}',\vec{k}) = \frac{2\pi}{\hbar}\frac{q^2\hbar\Xi_{ac}^2}{2\rho V\omega_q}\left(N_q + \frac{1}{2} \mp \frac{1}{2}\right)\underbrace{\delta(E_k - E_{k'} \mp \hbar\omega_q)\,\delta(\vec{k}' \pm \vec{q} - \vec{k})}$$

combined into single δ-function also lead to a factor $m^*/(\hbar^2 kq)$ and limits on the wavevector q:

$$0 \le q \le 2k\left(1 \mp \frac{v_s}{v}\right)$$

(Note the change in sign on the upper bound).

Therefore:

$$\left.\frac{\partial f_0}{\partial t}\right|_{coll} = \sum_q \frac{\pi q^2\Xi_{ac}^2}{\rho V v_s q}\Big[N_q f_0(E_k - \hbar\omega_q)\,\delta()\delta() + (N_q+1) f_0(E_k + \hbar\omega_q)\,\delta()\delta() - N_q f_0(E_k)\,\delta()\delta() - (N_q+1) f_0(E_k)\,\delta()\delta()\Big]$$

$$= \frac{V}{4\pi(2\pi)^3}\cdot 2\pi\frac{\pi\Xi_{ac}^2}{\rho V v_s}\frac{m^*}{\hbar^2 k}\left\{\int_0^{2k(1-v_s/v)} N_q f_0(E_k - \hbar\omega_q)\,q^2 dq + \int_0^{2k(1+v_s/v)}(N_q+1) f_0(E_k + \hbar\omega_q)\,q^2 dq - f_0(E_k)\int_0^{2k(1+v_s/v)} N_q\,q^2 dq - f_0(E_k)\int_0^{2k(1-v_s/v)}(N_q+1)\,q^2 dq\right\}$$

$$\left.\frac{\partial f_0}{\partial t}\right|_{coll} = \frac{m^* \Xi_{ac}^2}{4\pi \rho v_s \hbar^2 k} \Bigg\{ \underbrace{\int_0^{2k(1-v_s/v)} N_q \left[f_0(E_k - \hbar\omega_q) - f_0(E_k)\right] q^2 dq}_{I_1} +$$

$$+ \underbrace{\int_0^{2k(1+v_s/v)} N_q \left[f_0(E_k + \hbar\omega_q) - f_0(E_k)\right] q^2 dq}_{I_2} + \underbrace{\int_0^{2k(1+v_s/v)} f_0(E_k + \hbar\omega_q)\, q^2 dq}_{I_{3a}} -$$

$$- \underbrace{\int_0^{2k(1-v_s/v)} f_0(E_k)\, q^2 dq}_{I_{3b}}$$

The next task is to evaluate all these integrals. As we said earlier, we assume that the phonons are in equilibrium. Furthermore, if we are in the high-temperature limit, then:

$$f_0(E \pm \hbar\omega_q) \simeq f_0(E) \pm \hbar\omega_q \frac{\partial f_0}{\partial E} + \frac{1}{2}(\hbar\omega_q)^2 \frac{\partial^2 f_0}{\partial E^2}$$

This will be valid as long as $T > \hbar\omega/k_B$. In this limit the integral terms I_{3a} and I_{3b} become:

$$I_{3a} - I_{3b} \cong \int_0^{2k(1+v_s/v)} f_0(E_k) q^2 dq - \int_0^{2k(1-v_s/v)} f_0(E_k) q^2 dq +$$

$$+ \frac{\partial f_0}{\partial E_k} \int_0^{2k(1+v_s/v)} \hbar v_s q\, q^2 dq + \underbrace{\frac{1}{2}\frac{\partial^2 f_0}{\partial E_k^2} \int_0^{2k(1+v_s/v)} \hbar^2 v_s^2 q^2 q^2 dq}_{\text{this term is ignored since it involves } v_s^2.}$$

$$\approx f_0(E_k) \left.\frac{q^3}{3}\right|_{2k(1-v_s/v)}^{2k(1+v_s/v)} + \hbar v_s \frac{\partial f_0}{\partial E_k} \left.\frac{q^4}{4}\right|_0^{2k(1+v_s/v)}$$

$$\approx f_0(E_k)\frac{1}{3} 8k^3 \underbrace{\left[\left(1+\frac{v_s}{v}\right)^3 - \left(1-\frac{v_s}{v}\right)^3\right]}_{\approx 1 + 3\frac{v_s}{v} - 1 + 3\frac{v_s}{v} \approx 6\frac{v_s}{v}} + \hbar v_s \frac{\partial f_0}{\partial E_k}\frac{1}{4} \overset{4}{\cancel{16}} k^4 \underbrace{\left(1+\frac{v_s}{v}\right)^4}_{\approx 1}$$

$$\approx f_0(E_k)\frac{1}{\cancel{3}} 8k^3 \cdot \overset{2}{\cancel{6}} \frac{v_s}{v} + 4\hbar v_s \frac{\partial f_0}{\partial E_k} k^4 \approx 16 f_0 \frac{k^3 v_s}{v} + 4\hbar v_s \frac{\partial f_0}{\partial E_k} k^4$$

Now using: $m^* v = \hbar k$, we have: $\frac{k^3 v_s}{v} = \frac{k^3 v_s}{\hbar k} m^* = \frac{m^*}{\hbar} k^2 v_s$.
Then:

$$I_{3a} - I_{3b} \approx 16 \frac{m^*}{\hbar} v_s k^2 f_0 + 4 \hbar v_s \frac{\partial f_0}{\partial E_K} k^4$$

$$\approx 16 \frac{m^*}{\hbar} v_s \frac{2 m^* E_K}{\hbar^2} f_0 + 4 \cancel{\hbar} v_s \frac{\partial f_0}{\partial E_K} \frac{4 m^{*2} E_K^2}{\hbar^{\cancel{4}\,3}}$$

$$\approx \frac{32 m^{*2} v_s}{\hbar^3} f_0 E_K + \frac{16 m^{*2} v_s}{\hbar^3} E_K^2 \frac{\partial f_0}{\partial E_K}$$

The integral term I_1 is, in these limits, of the form:

$$I_1 = \int_0^{2k(1-v_s/v)} \underset{\uparrow\ \frac{k_BT}{\hbar\omega_q}}{N_q} \left[\cancel{f_0(E_K)} - \hbar\omega_q \frac{\partial f_0}{\partial E} + \frac{1}{2} (\hbar\omega_q)^2 \frac{\partial^2 f_0}{\partial E^2} - \cancel{f_0(E_K)} \right] q^2 dq$$

$$\approx \int_0^{2k(1-v_s/v)} \frac{k_BT}{\hbar\omega_q} \left[-\hbar\omega_q \frac{\partial f_0}{\partial E} + \frac{1}{2} (\hbar\omega_q)^2 \frac{\partial^2 f_0}{\partial E^2} \right] q^2 dq$$

$$\approx -k_BT \frac{\partial f_0}{\partial E} \int_0^{2k(1-v_s/v)} q^2 dq + \frac{k_BT}{2} \hbar v_s \frac{\partial^2 f_0}{\partial E^2} \int_0^{2k(1-v_s/v)} q^3 dq$$

$$\approx -k_BT \frac{\partial f_0}{\partial E} \cdot \frac{1}{3} 8k^3 (1 - v_s/v)^3 + \frac{k_BT \hbar v_s}{2} \frac{\partial^2 f_0}{\partial E^2} \frac{1}{\cancel{4}} \overset{4}{\cancel{16}} k^4 (1 - v_s/v)^4$$

$$\simeq -k_BT \frac{\partial f_0}{\partial E} \frac{8k^3}{3} \left(1 - 3\frac{v_s}{v}\right) + \frac{k_BT}{\cancel{2}} \hbar v_s \frac{\partial^2 f_0}{\partial E^2} \overset{2}{\cancel{4}} k^4$$

In the same manner, we can directly write that integral I_2 equals to:

$$I_2 \approx k_BT \frac{\partial f_0}{\partial E} \frac{8k^3}{3} \left(1 + \frac{3 v_s}{v}\right) + 2 k_BT \hbar v_s \frac{\partial^2 f_0}{\partial E^2} k^4$$

Hence:

$$I_1 + I_2 \approx k_BT \frac{\partial f_0}{\partial E} \frac{8k^{\cancel{3}\,2}}{\cancel{3}} \cdot \overset{2}{\cancel{6}} \frac{v_s m^*}{\hbar k} + 4 k_BT \hbar v_s k^4 \frac{\partial^2 f_0}{\partial E^2}$$

$$I_1 + I_2 \approx 16 k_B T \frac{m^* v_s}{\hbar} k^2 \frac{\partial f_0}{\partial E} + 4 k_B T \hbar v_s k^4 \frac{\partial^2 f_0}{\partial E^2}$$

$$\approx 16 k_B T \frac{m^* v_s}{\hbar} \frac{2m^* E_K}{\hbar^2} \frac{\partial f_0}{\partial E_K} + 4 k_B T \hbar v_s \frac{4 m^{*2} E_K^2}{\hbar^4} \frac{\partial^2 f_0}{\partial E_K^2}$$

$$\approx 32 k_B T \frac{m^{*2} v_s}{\hbar^3} E_K \frac{\partial f_0}{\partial E_K} + 16 K_B T \frac{m^{*2} v_s}{\hbar^3} E_K^2 \frac{\partial^2 f_0}{\partial E_K^2}$$

When all of the above results for the integrals are substituted back into the original expression for $(\partial f_0/\partial t)|_{coll}$, they give:

$$\left.\frac{\partial f_0}{\partial t}\right|_{coll} = \frac{m^* \Xi_{ac}^2}{4\pi \rho v_s \hbar^2} \frac{\hbar}{\sqrt{2m^* E}} \cancel{32}^{\,8} \frac{m^{*2} v_s E}{\hbar^3} \left\{ f_0(E) + \frac{E}{2} \frac{\partial f_0}{\partial E} + \right.$$

$$\left. + k_B T \frac{\partial f_0}{\partial E} + \frac{K_B T}{2} E \frac{\partial^2 f_0}{\partial E^2} \right\}$$

The constant in front of the parenthesis equals to:

$$a = \cancel{8}^{\,4} \frac{m^* \Xi_{ac}^2}{\pi \rho v_s \hbar} \frac{\sqrt{2m^*}}{2m^* \sqrt{E}} \frac{m^{*2} v_s E}{\hbar^3} = \frac{4 \Xi_{ac}^2 m^{*2} \sqrt{2m^* E}}{\pi \rho \hbar^4}$$

$$= 4 \Xi_{ac}^2 m^{*2} \sqrt{2m^* E} \frac{v_s^2}{L m^{*2} \Xi_{ac}^2 k_B T} = \frac{4 v_s^2}{L k_B T} \sqrt{2m^* E}$$

Therefore:

$$\boxed{\left.\frac{\partial f_0}{\partial t}\right|_{coll} = \frac{4 v_s^2}{L k_B T} \sqrt{2m^* E} \left\{ f_0(E) + \frac{E}{2} \frac{\partial f_0}{\partial E} + k_B T \frac{\partial f_0}{\partial E} + E \frac{k_B T}{2} \frac{\partial^2 f_0}{\partial E^2} \right\}} \quad (6)$$

↖ vanishes in equilibrium

- Combining now the results given in (5) and (6) gives:

$$-\frac{\cancel{2} L}{3\sqrt{2m^* E}} (e \mathcal{E}_z)^2 \left(\frac{\partial f_0}{\partial E} + E \frac{\partial^2 f_0}{\partial E^2} \right) = \frac{\cancel{4}^{\,2} v_s^2 \sqrt{2m^* E}}{L k_B T} \left\{ f_0 + \frac{E}{2} \frac{\partial f_0}{\partial E} + K_B T \frac{\partial f_0}{\partial E} + E k_B T \frac{\partial^2 f_0}{\partial E^2} \right\}$$

$$-\frac{(e \mathcal{E}_z)^2 L^2 k_B T}{6 v_s^2 (2m^* E)} \left(\frac{\partial f_0}{\partial E} + E \frac{\partial^2 f_0}{\partial E^2} \right) = f_0 + \frac{E}{2} \frac{\partial f_0}{\partial E} + k_B T \frac{\partial f_0}{\partial E} + E \frac{k_B T}{2} \frac{\partial^2 f_0}{\partial E^2}$$

Making the following change of variables: $y = E/k_BT$ and multiplying this last expression by 2E gives:

$$-\frac{(e\mathcal{E}_z L)^2}{6 v_s^2 m^*} k_BT\left(\frac{1}{k_BT}\frac{\partial f_0}{\partial y} + \frac{k_BT\, y}{(k_BT)^2}\frac{\partial^2 f_0}{\partial y^2}\right) =$$

$$= 2k_BT\, y\left(f_0 + \frac{k_BT\, y}{2k_BT}\frac{\partial f_0}{\partial y} + \frac{k_BT}{k_BT}\frac{\partial f_0}{\partial y} + \frac{(k_BT)^2 y}{2(k_BT)^2}\frac{\partial^2 f_0}{\partial y^2}\right)$$

$$-\frac{(eL)^2\mathcal{E}_z^2}{6m^* k_BT v_s^2}\left(f_0' + y f_0''\right) = 2y f_0 + \frac{2y^2}{2} f_0' + 2y f_0' + \frac{2y^2}{2} f_0''$$

$$-\alpha\left(f_0' + y f_0''\right) = 2y f_0 + y^2 f_0' + 2y f_0' + y^2 f_0''$$

$$(y^2 + \alpha y) f_0'' + (y^2 + 2y + \alpha) f_0' + 2y f_0 = 0$$

$$\boxed{\left(y + \frac{\alpha}{y}\right) f_0'' + \left(y + 2 + \frac{\alpha}{y}\right) f_0' + 2 f_0 = 0} \quad (7)$$

where we have defined $\alpha = \mathcal{E}_z^2/\mathcal{E}_1^2$ and $\mathcal{E}_1 = \frac{(6m^* k_BT v_s^2)^{1/2}}{eL}$

is the characteristic electric field. Note that the variable y is the reduced carrier energy.

- The differential equation given in (7) possesses an exact solution, the so-called Druyvesten distribution

$$f_0(y) = A(y+\alpha)^{\alpha} e^{-y}$$

where the constant A is normalization constant such that particle conservation is satisfied, i.e.

$$n = \int_0^{\infty} dE\, g_{3D}(E) f_0(E) \quad ; \quad g_{3D}(E) \text{ is the 3D-DOS function.}$$

- We now want to examine the behavior of this distribution function for both low-field ($\alpha \to 0$) and high-field (α large) conditions.

To examine the shape of the symmetric component of the distribution function at both low and high fields, it is convenient to write the differential equation given in (7) as:

$$\frac{1}{y}\frac{d}{dy}\left[y(\alpha+y)\frac{\partial f_0}{\partial y}+y^2 f_0\right]=0$$

Integrating once this equation gives:

$$\boxed{y(\alpha+y)\frac{\partial f_0}{\partial y}+y^2 f_0=0} \; (=c)$$

The constant c is taken to be zero

(a) Low-field condition:

For very low electric fields, $\alpha = \mathcal{E}_2^2/\mathcal{E}_1^2 \to 0$, and in this case, the differential equation simplifies to:

$$y^2\frac{\partial f_0}{\partial y}+y^2 f_0=0 \;\Rightarrow\; \frac{df_0}{dy}+f_0=0$$

This can be solved immediately using separation of variables, i.e.

$$\frac{df_0}{f_0}=-dy \;\Rightarrow\; f_0=Ae^{-y}=\underline{Ae^{-E/k_BT}}$$

Thermal distribution function

This result justifies the use of the equilibrium distribution function in the Low-field RTA. In addition, when substituted back into (6) it also gives: $(\partial f_0/\partial t)|_{coll}=0$.

(b) High-field condition:

When we have high electric field, then $\alpha \gg y$, and in this case we need to solve the following differential equation:

$$\alpha y\frac{df_0}{dy}+y^2 f_0=0 \;\Rightarrow\; \frac{df_0}{dy}=-\frac{y}{\alpha}f_0 \;\Rightarrow\; f_0(y)=Ae^{-y^2/2\alpha}$$

Therefore, at high electric fields, the distribution function tends towards:

$$f_0(E)=Ae^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}$$

If proper normalization is done, then:

$$f_0\left(\frac{E}{k_BT}\right)=f_0(y)=\frac{\bar{v}^2 n\hbar^3}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^*k_BT)^{3/2}}\,\alpha^{-3/4}e^{-y^2/2\alpha}$$

Hence, the energy distribution function is Gaussian rather than exponential in this limit. It is known as Druyrestyn distribution function, well known in plasma physics.

CONDUCTIVITY

The conductivity of the sample is evaluated by calculating the current density, i.e.

$$\vec{J} = -e\frac{2}{(2\pi)^3}\iiint d^3k\,\vec{v}\,f = -\frac{2e}{(2\pi)^3}\,2\pi\int_{-1}^{1} d(\cos\theta)\int_0^\infty k^2 dk\,\vec{v}\,f$$

When the electric field is along the z-axis, the z-component of the current density equals to:

$$J_z = -\frac{2e}{4\pi^2}\int_{-1}^{1} d(\cos\theta)\int_0^\infty k^2 dk\; v_z\left[\cancel{f_0}(E) + k_z\,g_1(E)\right]$$

0 (symmetric function → gives zero contribution to the current)

For parabolic bands, we have : $E = \frac{\hbar^2 k^2}{2m^*}$, which gives:

$$dE = \frac{\hbar^2}{m^*}k\,dk \quad \text{or:} \quad k\,dk = \frac{m^*}{\hbar^2}dE \quad \text{and} \quad k^2 dk = \frac{m^*}{\hbar^2}\sqrt{\frac{2m^*}{\hbar^2}E}\,dE$$

$$= \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}\,dE$$

Therefore:

$$J_z = -\frac{2e}{4\pi^2}\int_{-1}^{1} d(\cos\theta)\int_0^\infty \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\hbar}{m^*}\,k^2\cos^2\theta\,g_1(E)\sqrt{E}\,dE$$

$$= -\frac{\cancel{2}e}{\cancel{4}\pi^2}\,\frac{\hbar}{m^*}\,\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\underbrace{\int_{-1}^{1}\cos^2\theta\,d(\cos\theta)}_{\cancel{2}/3}\int_0^\infty \sqrt{E}\,g_1(E)\,dE\,k^2$$

$$= -\frac{e\hbar}{3m^*}\int_0^\infty \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E}\,g_1(E)\,dE\,k^2 =$$

$$= -\frac{e\hbar}{3m^*}\int_0^\infty g_{3D}(E)\,k^2\,g_1(E)\,dE$$

where: $g_1(E) = e\,\mathcal{E}_z\frac{\hbar}{m^*}\tau_m(E)\frac{\partial f_0}{\partial E} = e\,\mathcal{E}_z\frac{\hbar}{m^*}\sqrt{\frac{m^*}{2E}}\;L\;\frac{\partial f_0}{\partial E}$

For high electric fields:

$$f_0(E)=\frac{\bar{u}^2 n \hbar^3 \alpha^{-3/4}}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^* k_B T)^{3/2}}\, e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}$$

and:

$$\frac{\partial f_0}{\partial E}=\frac{\bar{u}^2 n \hbar^3 \alpha^{-3/4}}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^* k_B T)^{3/2}}\left(-\frac{1}{\cancel{2}\alpha}\right)\frac{\cancel{2}E}{(k_BT)^2}\, e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}$$

$$=-\frac{\bar{u}^2 n \hbar^3 E\ \alpha^{-3/4}}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^* k_B T)^{3/2}\alpha (k_BT)^2}\, e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}$$

Therefore:

$$g_1(E)=-e\,\varepsilon_z\,\frac{\hbar}{\sqrt{2m^*}\,\cancel{\sqrt{E}}}\,L\,\frac{\bar{u}^2 n \hbar^3 \overset{\sqrt{E}}{\cancel{E}}\ \alpha^{-3/4}}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^* k_B T)^{3/2}\alpha (k_BT)^2}\, e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}$$

and:

$$J_z=+\frac{e\cancel{\hbar}}{3\cancel{m^*}}\,\frac{2\cancel{m^*}}{\cancel{\hbar^2}}\,\frac{1}{\cancel{2}\cancel{\bar{u}^2}}\,\frac{\cancel{2}m^*\cancel{\sqrt{2m^*}}}{\cancel{\hbar^3}}\,e\,\varepsilon_z\,\frac{\cancel{\hbar}L}{\cancel{\sqrt{2m^*}}}\,\frac{\cancel{\bar{u}^2} n \cancel{\hbar^3}\alpha^{-3/4}}{2^{1/4}\,\Gamma\left(\frac{3}{4}\right)(m^* k_B T)^{3/2}\alpha (k_BT)^2}\cdot\int_0^\infty E^2 e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}dE$$

$$=\frac{2e^2\cancel{m^*}\varepsilon_z L n\,\alpha^{-3/4}}{3\cdot 2^{1/4}\,\Gamma\left(\frac{3}{4}\right)\cancel{m^*}k_BT\sqrt{m^*}\sqrt{k_BT}}\,\frac{1}{\alpha (k_BT)^2}\int_0^\infty E^2 e^{-\frac{1}{2\alpha}\left(\frac{E}{k_BT}\right)^2}dE$$

Using variable change: $x=\frac{E}{\sqrt{2\alpha}\,k_BT}$ we get $E=\sqrt{2\alpha}\,k_BT\,x$, i.e.

$$J_z=\frac{2e^2\varepsilon_z L n\,\alpha^{-3/4}}{3\cdot 2^{1/4}\cdot\Gamma\left(\frac{3}{4}\right)\sqrt{m^*}\,k_BT\cancel{\sqrt{k_BT}}}\,\frac{1}{\cancel{\alpha(k_BT)^2}}\cdot 2\cancel{\alpha}\cancel{(k_BT)^2}\sqrt{2}\sqrt{\alpha}\cancel{(k_BT)}^2\int_0^\infty x^2 e^{-x^2}dx$$

$$=\frac{4\sqrt{2}\,e^2\varepsilon_z L n}{3\cdot 2^{1/4}\,\Gamma\left(\frac{3}{4}\right)\sqrt{m^*}\sqrt{k_BT}\,\alpha^{1/4}}\int_0^\infty x^2 e^{-x^2}dx$$

where $\alpha^{1/4}=\sqrt{\frac{\varepsilon_z}{\varepsilon_1}}=\frac{1}{\varepsilon_1}\sqrt{\varepsilon_1\varepsilon_z}=\left[\frac{eL}{(6m^*k_BT v_s^2)^{1/2}}\right]^{-1}\sqrt{\varepsilon_1\varepsilon_z}=$

$$\alpha^{1/4}=\frac{\sqrt{6m^*k_BT\,v_s^2}}{eL}\sqrt{\varepsilon_1\varepsilon_z}$$

Using these results, we finally get:

$$J_z = \frac{\cancel{4}\sqrt{2}\, e^2 n L \mathcal{E}_z}{3\cdot 2^{1/4}\,\Gamma(\frac{3}{4})\sqrt{m^* k_B T}} \sqrt{\frac{\mathcal{E}_1}{\mathcal{E}_z}} \cdot \frac{1}{\cancel{4}}\sqrt{\pi} = \frac{\sqrt{2\pi}\, e^2 n L \cancel{\mathcal{E}_z}}{3\cdot 2^{1/4}\,\Gamma(\frac{3}{4})\sqrt{m^* k_B T}} \sqrt{\frac{\mathcal{E}_1}{\mathcal{E}_z}} = \sigma\, \cancel{\mathcal{E}_z}$$

where we have used:

$$\int_0^\infty x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{4}$$

The conductivity is given by:

$$\boxed{\sigma(\mathcal{E}_z) = \frac{\sqrt{2\pi}\; n e^2 L}{3\cdot 2^{1/4}\,\Gamma(\frac{3}{4})\sqrt{m^* k_B T}} \sqrt{\frac{\mathcal{E}_1}{\mathcal{E}_z}}}$$ High-field result

The low-field conductivity is obtained using : $f_0(E) = A e^{-E/k_BT}$, which gives:

$$\frac{\partial f_0}{\partial E} = -\frac{A}{k_BT} e^{-E/k_BT}$$

i.e. $$g_1(E) = e\mathcal{E}_z \frac{\hbar}{\sqrt{2m^*E}} L \left(-\frac{A}{k_BT}\right) e^{-E/k_BT}$$

Substituting back into the expression for J_z we have:

$$J_z = -\frac{e\hbar}{3m^*}\int_0^\infty a\cancel{\sqrt{E}}\, e\mathcal{E}_z \frac{\hbar}{\sqrt{2m^*\cancel{E}}} \frac{2m^*E}{\hbar^2} L\left(-\frac{A}{k_BT}\right) e^{-E/k_BT} dE$$

$$= -\frac{e^2\cancel{\hbar^2}\cdot 2\cancel{m^*} a\, \mathcal{E}_z L}{3\cancel{m^*}\sqrt{2m^*}\,\cancel{\hbar^2}}\left(-\frac{A}{k_BT}\right)\int_0^\infty E\, e^{-E/k_BT} dE \qquad , x = E/k_BT$$

$$= +\frac{2e^2 a\,\mathcal{E}_z L A}{3\sqrt{2m^*}\,k_BT}(k_BT)^2\int_0^\infty x e^{-x} dx =$$

$$= \frac{2e^2\cancel{a}\,\mathcal{E}_z L \cancel{A}}{3\sqrt{2m^*}}(k_BT)\, n \frac{\int_0^\infty x e^{-x} dx}{\cancel{A}\cancel{a}\int_0^\infty E^{1/2} e^{-E/k_BT} dE} = \frac{2e^2\mathcal{E}_z L n \cancel{k_BT}\int_0^\infty x e^{-x} dx}{3\sqrt{2m^*}\,\cancel{k_BT}\sqrt{k_BT}\int_0^\infty x^{1/2} e^{-x} dx}$$

$$\int_0^\infty x^n e^{-\mu x}\,dx = \frac{n!}{\mu^{n+1}}, \quad \mu > 0$$

$$\int_0^\infty x^{n-\frac{1}{2}} e^{-\mu x}\,dx = \sqrt{\pi}\,\frac{1}{2}\cdot\frac{3}{2}\cdots\frac{(2n-1)}{2}\,\frac{1}{\mu^{n+1/2}}$$

Therefore:

$$\int_0^\infty x e^{-x}\,dx = \frac{1!}{1^2} = 1$$

$$\int_0^\infty x^{1/2} e^{-x}\,dx = \sqrt{\pi}\,\frac{1}{2} = \frac{\sqrt{\pi}}{2}$$

$$J_z = \frac{2e^2 \mathcal{E}_z L n}{3\sqrt{2}\,\sqrt{m^* k_B T}}\,\frac{2}{\sqrt{\pi}} = \frac{(8/\pi)^{1/2}\, n e^2 L}{3\,(m^* k_B T)^{1/2}}\,\mathcal{E}_z = \sigma_0\,\mathcal{E}_z$$

The low-field conductivity is given by:

$$\boxed{\sigma_0 = \frac{(8/\pi)^{1/2}\, n e^2 L}{3\,(m^* k_B T)^{1/2}}}$$ Low-field expression for the conductivity

Thus: $$\frac{n e^2 L}{(m^* k_B T)^{1/2}} = \frac{3\sigma_0}{(8/\pi)^{1/2}} = \frac{3\sigma_0}{2\sqrt{2}/\sqrt{\pi}} = \frac{3\sqrt{\pi}\,\sigma_0}{2\sqrt{2}}$$

or:

$$\sigma(\mathcal{E}_z) = \frac{\sqrt{2\pi}}{\cancel{3}\cdot 2^{1/4}\,\Gamma(3/4)}\cdot\frac{\cancel{3}\sqrt{\pi}\,\sigma_0}{2\cancel{\sqrt{2}}}\sqrt{\frac{\mathcal{E}_1}{\mathcal{E}_z}} = \sigma_0\,\frac{\pi}{2^{5/4}\,\Gamma(3/4)}\cdot\sqrt{\frac{\mathcal{E}_1}{\mathcal{E}_z}}$$

Note:
- The above-described calculation is based on a model with only a single set of carriers associated with one valley, and with a scattering determined by acoustic phonons. To compare with experiments, one also needs to consider scattering by optical and intervalley phonons. The latter is of highest importance under high-field conditions, since the electric field might raise the electrons to rather high temperatures.
- This example also illustrates the mathematical difficulties associated with the analytical approaches. To obtain mobility under hot-electron (high-field) conditions, it is much easier to use the Monte Carlo method.