Problem #2:

Using Rode's iterative method, we need to compute the mobility as a function of the impurity concentration for n-type GaAs at T=300 K. Scattering mechanisms included in the model are:

- acoustic deformation potential scattering, for which the elastic and equipartition approximation is valid and $\Xi_{ac} = 7.01\,eV$ and $v_s = 5.22\times10^3$ m/s
- Polar optical phonon scattering for which $\hbar\omega_{LO} = 35.36\,meV$
- Coulomb scattering treated within the Brooks-Herring approach.

(A) Coulomb scattering:

- For Coulomb scattering, the matrix element squared for scattering between states $\vec{k}$ and $\vec{k}'$ due to a single charged impurity is:

$$|M(\vec{k},\vec{k}')|^2 = \left[\frac{e^2}{K_s\varepsilon_0 V}\,\frac{1}{q^2+1/L_D^2}\right]^2 \delta(\vec{k}-\vec{k}'-\vec{q})$$

where $\vec{q} = \vec{k}-\vec{k}'$ is the momentum transfer in the scattering process, and L_D is the Debye screening length that is calculated using

$$L_D = \sqrt{\frac{K_s\varepsilon_0 V_T}{en}}$$

for non-degenerate semiconductors, where $V_T = k_B T/e$ is the thermal voltage. The transition rate from state $\vec{k}$ to state $\vec{k}'$ is then given by:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\,\frac{e^4}{(K_s\varepsilon_0)^2V^2}\,N_I\,\frac{1}{(q^2+1/L_D^2)^2}\,\delta(\vec{k}-\vec{k}'-\vec{q})\,\delta(E_k-E_{k'})$$

where N_I is the total number of impurities in volume V that are assumed to be uniformly distributed and

$$n_I = \frac{N_I}{V} \quad \text{is the impurity concentration.}$$

Therefore:

$$S(\vec{k},\vec{k}') = \frac{2\pi}{\hbar}\left(\frac{e^2}{K_s\varepsilon_0}\right)^2\frac{n_I}{V}\,\frac{1}{(q^2+1/L_D^2)^2}\,\delta(\vec{k}-\vec{k}'-\vec{q})\,\delta(E_k-E_{k'})$$

If α is the angle between $\vec{k}$ and $\vec{k}'$, then:

$$q^2 = \vec{q}\cdot\vec{q} = (\vec{k}-\vec{k}')\cdot(\vec{k}-\vec{k}') = k^2+k'^2-2kk'\cos\alpha = 2k^2(1-\cos\alpha)$$

- The momentum relaxation rate for ionized impurity scattering equals to:

$$\frac{1}{\tau_m(k)} = \frac{V}{(2\pi)^3}\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\alpha) \int_0^{\infty} k'^2 dk' \; S(\vec{k},\vec{k}')\,(1-\cos\alpha)$$

$$= \frac{\cancel{V}}{(2\pi)^{\cancel{3}}}\, 2\pi \left(\frac{2\pi}{\hbar}\right)\left(\frac{e^2}{K_s\varepsilon_0}\right)^2 \frac{n_I}{\cancel{V}} \int_{-1}^{1} d(\cos\alpha)\int_0^{\infty} k'^2 dk' \; \frac{1-\cos\alpha}{(q^2+1/L_D^2)^2}\,\delta(E_k-E_{k'})\,\delta(\vec{k}-\vec{k}'-\vec{q})$$

$$= \frac{n_I e^4}{2\pi\hbar (K_s\varepsilon_0)^2}\int_{-1}^{1} d(\cos\alpha)\int_0^{\infty} k'^2 dk' \frac{1-\cos\alpha}{\left[2k^2(1-\cos\alpha)+1/L_D^2\right]^2}\,\delta(E_k-E_{k'})$$

For parabolic band structure, for which $E_{k'} = \hbar^2 k'^2/2m^*$, we have:

$$dE_{k'} = \frac{\hbar^2}{m^*} k' dk' \;\Rightarrow\; k' dk' = \frac{m^*}{\hbar^2} dE_{k'}$$

$$k'^2 dk' = k' k' dk' = \sqrt{\frac{2m^* E_{k'}}{\hbar^2}}\,\frac{m^*}{\hbar^2}\, dE_{k'} = \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_{k'}}\, dE_{k'}$$

With the above change of variables, the momentum relaxation rate becomes:

$$\frac{1}{\tau_m(k)} = \frac{n_I e^4}{2\pi\hbar (K_s\varepsilon_0)^2}\,\frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_{-1}^{1} d(\cos\alpha)\int_0^{\infty}\frac{1-\cos\alpha}{\left[2k^2(1-\cos\alpha)+1/L_D^2\right]^2}\sqrt{E_{k'}}\,\delta(E_k-E_{k'})\,dE_{k'}$$

$$= \frac{n_I e^4}{4\pi\hbar (K_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_k}\int_{-1}^{1}\frac{(1-\cos\alpha)\,d(\cos\alpha)}{\left[2k^2(1-\cos\alpha)+1/L_D^2\right]^2}$$

we now use the following change of variables:

$$x = 1-\cos\alpha \;\Rightarrow\; \begin{cases}\cos\alpha = -1, & x = 2\\ \cos\alpha = 1, & x = 0\end{cases}$$

Then:

$$\frac{1}{\tau_m(k)} = \frac{n_I e^4}{4\pi\hbar (K_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_k}\int_0^2 \frac{x\,dx}{(2k^2 x + 1/L_D^2)^2} = \frac{n_I e^4}{4\pi\hbar (K_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{E_k}}{(2k^2)^2}\int_0^2\frac{x\,dx}{\left(x+\frac{1}{2k^2L_D^2}\right)^2}$$

$$= \frac{n_I e^4}{4\pi\hbar (K_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{E_k}}{4k^4}\int_0^2 \frac{x+\frac{1}{2k^2L_D^2}-\frac{1}{2k^2L_D^2}}{\left(x+\frac{1}{2k^2L_D^2}\right)^2}\,dx =$$

$$= \frac{n_I e^4}{4\pi\hbar (K_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{E_k}}{4k^4}\left[\int_0^2\frac{dx}{x+\frac{1}{2k^2L_D^2}} - \frac{1}{2k^2L_D^2}\int_0^2\frac{dx}{\left(x+\frac{1}{2k^2L_D^2}\right)^2}\right]$$

$$\frac{1}{\tau_m(k)} = \frac{n_I e^4}{4\pi\hbar(\kappa_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{E_k}}{4k^4}\left[\ln\left|\frac{2+\frac{1}{2k^2L_D^2}}{\frac{1}{2k^2L_D^2}}\right| + \frac{1}{2k^2L_D^2}\,\frac{1}{x+\frac{1}{2k^2L_D^2}}\Bigg|_0^2\right]$$

$$= \frac{n_I e^4}{4\pi\hbar(\kappa_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{\sqrt{E_k}}{4k^4}\left[\ln\left(1+4k^2L_D^2\right) + \right.$$

$$\left. + \underbrace{\frac{1}{2k^2L_D^2}\left(\frac{1}{2+\frac{1}{2k^2L_D^2}} - 2k^2L_D^2\right)}\right]$$

$$\frac{1}{\cancel{2k^2L_D^2}}\,\frac{\cancel{2k^2L_D^2}}{1+4k^2L_D^2} - 1 = \frac{1}{1+4k^2L_D^2} - 1 = \frac{1-1-4k^2L_D^2}{1+4k^2L_D^2} = -\frac{4k^2L_D^2}{1+4k^2L_D^2}$$

$$\frac{1}{\tau_m(k)} = \underbrace{\frac{n_I e^4}{4\pi\hbar(\kappa_s\varepsilon_0)^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\frac{1}{4k^4}\left(\frac{\hbar^2k^2}{2m^*}\right)^{1/2}}\left[\ln\left(1+4k^2L_D^2\right) - \frac{4k^2L_D^2}{1+4k^2L_D^2}\right]$$

$$\frac{n_I e^4}{4\pi\hbar(\kappa_s\varepsilon_0)^2}\,\frac{2m^*\sqrt{2m^*}}{\hbar^3}\,\frac{1}{4k^{4}}\,\frac{\hbar k}{\sqrt{2m^*}} = \frac{n_I e^4 m^*}{8\pi\hbar^3k^3(\kappa_s\varepsilon_0)^2}$$

The final expression for the momentum relaxation rate is then:

$$\frac{1}{\tau_m(k)} = \frac{n_I e^4 m^*}{8\pi\hbar^3k^3(\kappa_s\varepsilon_0)^2}\left[\ln\left(1+4k^2L_D^2\right) - \frac{4k^2L_D^2}{1+4k^2L_D^2}\right]$$

where: $\gamma(k) = \gamma(E) = 4k^2L_D^2 = 4L_D^2\,\dfrac{2m^*E_k}{\hbar^2} = \dfrac{8m^*L_D^2E_k}{\hbar^2}$

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

The energy dependent momentum relaxation rate is, thus, given by:

$$\frac{1}{\tau_m(E)} = \frac{n_I e^4}{16\pi(\kappa_s\varepsilon_0)^2\sqrt{2m^*}}E^{-3/2}\left\{\ln\left[1+\gamma(E)\right] - \frac{\gamma(E)}{1+\gamma(E)}\right\}$$

where: $\gamma(E) = 8m^*L_D^2E/\hbar^2$.

(B) Acoustic phonon scattering

In the elastic and equipartition approximation, the acoustic phonon scattering is isotropic scattering process, which means that the scattering rate and the momentum relaxation rates are identical. Therefore, we can directly write the momentum relaxation rate for this scattering process, since it was derived in class, to be equal to:

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

(C) Total momentum relaxation rate due to elastic scattering processes

$$\boxed{\frac{1}{\tau_m^{el}(E)} = \frac{1}{\tau_m^{ac}(E)} + \frac{1}{\tau_m^{ii}(E)} = \frac{m^* \Xi_{ac}^2 k_B T \sqrt{2m^* E}}{\pi \hbar^4 \rho v_s^2} + \frac{n_I e^4 E^{-3/2}}{16\pi (\kappa_s \varepsilon_0)^2 \sqrt{2m^*}} \left\{ \ln[1+\gamma(E)] - \frac{\gamma(E)}{1+\gamma(E)} \right\}} \qquad (1)$$

where:

$$\gamma(E) = 8m^* L_D^2 E/\hbar^2 \quad \text{and} \quad L_D = \sqrt{\kappa_s \varepsilon_0 V_T/(en)} .$$

(D) Inelastic – Polar Optical Phonon Scattering

For the inelastic scattering processes, we need to evaluate the integrals of the form:

$$I_0(\vec{k}) = \sum_{\vec{k}'} \left\{ S^{in}(\vec{k}', \vec{k}) f_0(\vec{k}') + S^{in}(\vec{k}, \vec{k}') [1 - f_0(\vec{k}')] \right\}$$

$$\tilde{I}(\vec{k}) = \sum_{\vec{k}'} g(\vec{k}') \left\{ S^{in}(\vec{k}', \vec{k}) [1 - f_0(\vec{k})] + S^{in}(\vec{k}, \vec{k}') f_0(\vec{k}) \right\} \cos\alpha$$

Again, the angle α is between wavevectors $\vec{k}$ and $\vec{k}'$. The transition rates for polar optical phonon scattering from some initial state $\vec{k}$ to a final state $\vec{k}'$ and vice-versa are given by:

$$S(\vec{k}, \vec{k}') = \frac{2\pi}{\hbar} \frac{\hbar e^2 \omega_{LO}}{2Vq^2} \left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)} \right] \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{k} - \vec{k}' \pm \vec{q}) \delta(E_{k'} - E_k \mp \hbar\omega_{LO})$$

$$S(\vec{k}', \vec{k}) = \frac{\pi e^2 \omega_{LO}}{Vq^2} \left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)} \right] \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \delta(\vec{k}' - \vec{k} \pm \vec{q}) \delta(E_k - E_{k'} \mp \hbar\omega_{LO})$$

The term $I_0(k)$ becomes:

$$I_0(\vec{k}) = \frac{\pi e^2 \omega_{LO}}{\cancel{V}}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\cancel{V}}{(2\pi)^3}\,\cancel{2\pi}\,\times$$

$$\times\left\{\int_{-1}^{1} d(\cos\alpha)\int_0^\infty k'^2\,dk'\,\frac{1}{q^2}\left[f_0(k')\,\delta(\vec{k}' - \vec{k} \pm \vec{q})\,\delta(E_k - E_{k'} \mp \hbar\omega_{LO}) + \right.\right.$$

$$\left.\left. + \left[1 - f_0(k')\right]\delta(\vec{k} - \vec{k}' \pm \vec{q})\,\delta(E_{k'} - E_k \mp \hbar\omega_{LO})\right]\right\}$$

Again, using parabolic band structure, for which $E_{k'} = \hbar^2 k'^2/(2m^*)$, we have:

$$dE_{k'} = \frac{\hbar^2}{m^*}k'\,dk' \Rightarrow k'\,dk' = \frac{m^*}{\hbar^2}\,dE_{k'}$$

$$k'^2\,dk' = \sqrt{\frac{2m^* E_{k'}}{\hbar^2}}\;\frac{m^*}{\hbar^2}\,dE_{k'} = \frac{1}{2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E_{k'}}\,dE_{k'}$$

Also:
$$\frac{1}{q^2} = \frac{1}{|\vec{k} - \vec{k}'|^2} = \frac{1}{k^2 + k'^2 - 2kk'\cos\alpha}\left(\frac{2m^*}{\hbar^2}\right)\left(\frac{\hbar^2}{2m^*}\right)$$

$$= \frac{\hbar^2}{2m^*}\,\frac{1}{E_k + E_{k'} - 2\sqrt{E_k E_{k'}}\cos\alpha}$$

Substituting the above results into the expression for $I_0(k)$ gives:

$$I_0(k) = \frac{\cancel{\pi} e^2 \omega_{LO}}{4\pi^2 k}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right)\frac{\cancel{\hbar^2}}{\cancel{2m^*}}\,\frac{1}{2}\,\frac{\cancel{2m^*}}{\cancel{\hbar^2}}\sqrt{\frac{2m^*}{\hbar^2}}\,\times$$

$$\times\int_{-1}^{1} d(\cos\alpha)\int_0^\infty \frac{\sqrt{E_{k'}}\,dE_{k'}}{E_k + E_{k'} - 2\sqrt{E_k E_{k'}}\cos\alpha}\left\{f_0(E_{k'})\,\delta(E_k - E_{k'} \mp \hbar\omega_{LO}) + \right.$$

$$\left. + \left[1 - f_0(E_{k'})\right]\delta(E_{k'} - E_k \mp \hbar\omega_{LO})\right\}$$

$$= \frac{e^2 \omega_{LO}\sqrt{2m^*}}{8\pi\hbar}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right)\times$$

$$\times\left\{\int_{-1}^{1} d(\cos\alpha)\,\frac{f_0(E_k \mp \hbar\omega_{LO})\sqrt{E_k \mp \hbar\omega_{LO}}\;\theta(E_k \mp \hbar\omega_{LO})}{E_k + E_k \mp \hbar\omega_{LO} - 2\sqrt{E_k(E_k \mp \hbar\omega_{LO})}\cos\alpha} + \right.$$

$$\left. + \int_{-1}^{1} d(\cos\alpha)\,\frac{\left[1 - f_0(E_k \pm \hbar\omega_{LO})\right]\sqrt{E_k \pm \hbar\omega_{LO}}\;\theta(E_k \pm \hbar\omega_{LO})}{E_k + E_k \pm \hbar\omega_{LO} - 2\sqrt{E_k(E_k \pm \hbar\omega_{LO})}\cos\alpha}\right\}$$

Using the change of variables $x = \cos\alpha$, the integrals of the force below are:

$$A = \int_{-1}^{1} \frac{dx}{a+b-2\sqrt{ab}\,x} = \frac{1}{(-2\sqrt{ab})} \int_{-1}^{1} \frac{d(-2\sqrt{ab}\,x)}{a+b-2\sqrt{ab}\,x} =$$

$$= -\frac{1}{2\sqrt{ab}} \ln\left(a+b-2\sqrt{ab}\,x\right)\Big|_{-1}^{1} = -\frac{1}{2\sqrt{ab}} \ln\left|\frac{a+b-2\sqrt{ab}}{a+b+2\sqrt{ab}}\right| =$$

$$= +\frac{1}{2\sqrt{ab}} \ln\left|\frac{\sqrt{a}+\sqrt{b}}{\sqrt{a}-\sqrt{b}}\right|^2 = \frac{1}{\sqrt{ab}} \ln\left|\frac{\sqrt{a}+\sqrt{b}}{\sqrt{a}-\sqrt{b}}\right|$$

Therefore:

$$I_0(k) = \frac{e^2 \omega_{L0} \sqrt{2m^*}}{8\pi\hbar}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right) \times$$

$$\times \left\{ f_0(E_k \mp \hbar\omega_{L0}) \frac{\cancel{\sqrt{E_k \mp \hbar\omega_{L0}}}}{\sqrt{E_k(\cancel{E_k \mp \hbar\omega_{L0}})}} \,\Theta(E_k \mp \hbar\omega_{L0}) \ln\left|\frac{\sqrt{E_k} + \sqrt{E_k \mp \hbar\omega_{L0}}}{\sqrt{E_k} - \sqrt{E_k \mp \hbar\omega_{L0}}}\right| + \right.$$

$$\left. + \left[1 - f_0(E_k \pm \hbar\omega_{L0})\right] \frac{\cancel{\sqrt{E_k \pm \hbar\omega_{L0}}}\,\Theta(E_k \pm \hbar\omega_{L0})}{\sqrt{E_k(\cancel{E_k \pm \hbar\omega_{L0}})}} \ln\left|\frac{\sqrt{E_k} + \sqrt{E_k \pm \hbar\omega_{L0}}}{\sqrt{E_k} - \sqrt{E_k \pm \hbar\omega_{L0}}}\right| \right\}$$

$$\boxed{\begin{aligned} I_0(E_k) = {} & \frac{e^2 \omega_{L0} \sqrt{m^*}}{4\sqrt{2}\,\pi\hbar\sqrt{E_k}}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right) \times \\ & \times \left\{ f_0(E_k \mp \hbar\omega_{L0}) \ln\left|\frac{\sqrt{E_k} + \sqrt{E_k \mp \hbar\omega_{L0}}}{\sqrt{E_k} - \sqrt{E_k \mp \hbar\omega_{L0}}}\right| \Theta(E_k \mp \hbar\omega_{L0}) + \right. \\ & \left. + \left[1 - f_0(E_k \pm \hbar\omega_{L0})\right] \ln\left|\frac{\sqrt{E_k} + \sqrt{E_k \pm \hbar\omega_{L0}}}{\sqrt{E_k} - \sqrt{E_k \pm \hbar\omega_{L0}}}\right| \Theta(E_k \pm \hbar\omega_{L0}) \right\} \end{aligned}} \quad (1)$$

The integral $\tilde{I}(k)$ that was given in the class notes can also be rewritten in the following form:

$$\tilde{I}(k) = (1 - f_0)\sum_{k'} g(k')\, S^{in}(\vec{k}', \vec{k}) \cos\alpha + f_0(k) \sum_{k'} g(k')\, S^{in}(\vec{k}, \vec{k}') =$$

$$= \frac{\pi e^2 \omega_{L0}}{\cancel{V}}\left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)}\right]\left(N_0 + \frac{1}{2} \mp \frac{1}{2}\right) \frac{\cancel{V}}{(2\pi)^{\cancel{3}2}} \cancel{2\pi} \int_{-1}^{1} d(\cos\alpha) \int_0^\infty k'^2 dk' \cdot$$

$$\cdot \frac{\hbar^2}{2m^*} \cdot \frac{\cos\alpha}{E_k + E_{k'} - 2\sqrt{E_k E_{k'}}\cos\alpha} \left\{ [1 - f_0(k)]\, g(k')\, \delta(E_k - E_{k'} \mp \hbar\omega_{LO}) + \right.$$

$$\left. + f_0(k)\, g(k')\, \delta(E_{k'} - E_k \mp \hbar\omega_{LO}) \right\}$$

$$= \frac{\bar{v} e^2 \omega_{LO}}{4\bar{v}^2} \cancel{\frac{\hbar^2}{2m^*}} \frac{1}{2} \cancel{\frac{2m^*}{\hbar^2}} \frac{\sqrt{2m^*}}{\hbar} \left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)} \right] \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \times$$

$$\times \left\{ [1 - f_0(E_k)]\, g(E_k \mp \hbar\omega_{LO})\, \theta(E_k \mp \hbar\omega_{LO}) \int_{-1}^{1} \frac{x\,dx\, \sqrt{E_k \mp \hbar\omega_{LO}}}{E_k + E_k \mp \hbar\omega_{LO} - 2\sqrt{E_k(E_k \mp \hbar\omega_{LO})}\,x} + \right.$$

$$\left. + f_0(E_k)\, g(E_k \pm \hbar\omega_{LO})\, \theta(E_k \pm \hbar\omega_{LO}) \int_{-1}^{1} \frac{x\,dx\, \sqrt{E_k \pm \hbar\omega_{LO}}}{E_k + E_k \pm \hbar\omega_{LO} - 2\sqrt{E_k(E_k \pm \hbar\omega_{LO})}\,x} \right\}$$

$$= \frac{e^2 \omega_{LO} \sqrt{2m^*}}{8\bar{v}\hbar} \left[\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon(0)} \right] \left(N_0 + \frac{1}{2} \mp \frac{1}{2} \right) \{ \cdots \}$$

In this case, we need to evaluate integrals of the form:

$$B = \int_{-1}^{1} \frac{x\,dx}{a + b - 2\sqrt{ab}\,x} = -\frac{1}{2\sqrt{ab}} \int_{-1}^{1} \frac{-2\sqrt{ab}\,x\,dx}{a + b - 2\sqrt{ab}\,x} = -\frac{1}{2\sqrt{ab}} \int_{-1}^{1} \frac{a + b - 2\sqrt{ab}x - (a+b)}{a + b - 2\sqrt{ab}\,x}\,dx$$

$$= -\frac{1}{2\sqrt{ab}} \left\{ \int_{-1}^{1} dx - \frac{(a+b)}{(-2\sqrt{ab})} \int_{-1}^{1} \frac{dx\,(-2\sqrt{ab})}{a + b - 2\sqrt{ab}\,x} \right\} =$$

$$= -\frac{1}{2\sqrt{ab}} \left\{ 2 + \frac{a+b}{2\sqrt{ab}} \ln(a + b - 2x\sqrt{ab}) \Big|_{-1}^{1} \right\} =$$

$$= -\frac{1}{2\sqrt{ab}} \left\{ 2 + \frac{a+b}{2\sqrt{ab}} \ln \left| \frac{a + b - 2\sqrt{ab}}{a + b + 2\sqrt{ab}} \right| \right\} = -\frac{1}{\sqrt{ab}} + \frac{a+b}{4ab} \ln \left| \frac{a + b + 2\sqrt{ab}}{a + b - 2\sqrt{ab}} \right|$$

$$= -\frac{1}{\sqrt{ab}} + \frac{a+b}{2ab} \ln \left| \frac{\sqrt{a} + \sqrt{b}}{\sqrt{a} - \sqrt{b}} \right|$$

Then: $B' = \int_{-1}^{1} \frac{\sqrt{b}\,x\,dx}{a + b - 2\sqrt{ab}\,x} = -\frac{1}{\sqrt{a}} + \frac{a+b}{2a\sqrt{b}} \ln \left| \frac{\sqrt{a} + \sqrt{b}}{\sqrt{a} - \sqrt{b}} \right| = -\frac{1}{\sqrt{a}} \left[1 - \frac{a+b}{2\sqrt{ab}} \ln \left| \frac{\sqrt{a} + \sqrt{b}}{\sqrt{a} - \sqrt{b}} \right| \right]$

Substituting these results into the expression for $\bar{I}(k)$ finally leads to.

Therefore,

$$\frac{\partial f_0}{\partial E_k} = -\frac{1}{\left[1+\exp\left(\frac{E_k+E_c-E_F}{k_BT}\right)\right]^2}\frac{1}{k_BT}\exp\left(\frac{E_k+E_c-E_F}{k_BT}\right)$$

$$= -\frac{1}{k_BT}\frac{\exp\left(\frac{E_k+E_c-E_F}{k_BT}\right)}{\left[1+\exp\left(\frac{E_k+E_c-E_F}{k_BT}\right)\right]^2}$$

Assuming non-degenerate sc (which is not really true when $N_D > 5\times10^{17}\ cm^{-3}$ in GaAs materials), we have:

$$N_D = N_c \exp\left(\frac{E_F-E_c}{k_BT}\right) \Rightarrow \boxed{E_c - E_F = k_BT\ln\left(\frac{N_c}{N_D}\right)}$$

$$\boxed{\exp\left(\frac{E_c-E_F}{k_BT}\right) = \frac{N_c}{N_D}}$$

To summarize:

$$\frac{\partial f_0}{\partial E_k} = -\frac{1}{k_BT}\frac{N_c}{N_D}\frac{\exp(E_k/k_BT)}{\left[1+\frac{N_c}{N_D}\exp\left(\frac{E_k}{k_BT}\right)\right]^2}$$

$$g_{n+1}(E_k) = \frac{\tilde{I}_n(E_k) + e\mathcal{E}\sqrt{\frac{2E_k}{m^*}}\left(\partial f_0/\partial E_k\right)}{I_0(E_k) + \frac{1}{\tau_m^{el}(E_k)}}$$ $\rightarrow$ need to iterate until convergence

The low-field electron mobility is then calculated using:

$$\mu_n = -\frac{1}{3}\frac{\int_0^\infty E^{1/2}\left[v(E)g(E)/\mathcal{E}\right]dE}{\int_0^\infty E^{1/2} f_0(E)\,dE}$$

$$\tilde{I}(E_k) = \frac{e^2\omega_{LO}\sqrt{2m^*}}{8\pi\hbar\sqrt{E_k}}\left[\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon(0)}\right]\left(N_0+\frac{1}{2}\mp\frac{1}{2}\right)\times$$

$$\times\left\{\left[1-f_0(E_k)\right]g(E_k\mp\hbar\omega_{LO})\,\theta(E_k\mp\hbar\omega_{LO})\left[\frac{E_k\mp\hbar\omega_{LO}+E_k}{2\sqrt{E_k(E_k\mp\hbar\omega_{LO})}}\ln\left|\frac{\sqrt{E_k}+\sqrt{E_k\mp\hbar\omega_{LO}}}{\sqrt{E_k}-\sqrt{E_k\mp\hbar\omega_{LO}}}\right|-1\right]\right.$$

$$\left.+f_0(E_k)\,g(E_k\pm\hbar\omega_{LO})\,\theta(E_k\pm\hbar\omega_{LO})\left[\frac{E_k+E_k\pm\hbar\omega_{LO}}{2\sqrt{E_k(E_k\pm\hbar\omega_{LO})}}\ln\left|\frac{\sqrt{E_k}+\sqrt{E_k\pm\hbar\omega_{LO}}}{\sqrt{E_k}-\sqrt{E_k\pm\hbar\omega_{LO}}}\right|-1\right]\right\}$$

or:

$$\boxed{\begin{aligned}\tilde{I}(E_k) &= \frac{e^2\omega_{LO}\sqrt{m^*}}{4\sqrt{2}\pi\hbar\sqrt{E_k}}\left[\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon(0)}\right]\left(N_0+\frac{1}{2}\mp\frac{1}{2}\right)\times \qquad (3)\\ &\times\left\{\left[1-f_0(E_k)\right]g(E_k\mp\hbar\omega_{LO})\,\theta(E_k\mp\hbar\omega_{LO})\left[\frac{2E_k\mp\hbar\omega_{LO}}{2\sqrt{E_k(E_k\mp\hbar\omega_{LO})}}\ln\left|\frac{\sqrt{E_k}+\sqrt{E_k\mp\hbar\omega_{LO}}}{\sqrt{E_k}-\sqrt{E_k\mp\hbar\omega_{LO}}}\right|-1\right]\right.\\ &\left.+f_0(E_k)\,g(E_k\pm\hbar\omega_{LO})\,\theta(E_k\pm\hbar\omega_{LO})\left[\frac{2E_k\pm\hbar\omega_{LO}}{2\sqrt{E_k(E_k\pm\hbar\omega_{LO})}}\ln\left|\frac{\sqrt{E_k}+\sqrt{E_k\pm\hbar\omega_{LO}}}{\sqrt{E_k}-\sqrt{E_k\pm\hbar\omega_{LO}}}\right|-1\right]\right\}\end{aligned}}$$

- Now, using the results given in (1), (2) and (3), we can calculate the updated function $g(E_k)$ using:

$$g_{n+1}(E_k) = \frac{\tilde{I}_n(E_k) + e v \mathcal{E}\left(\frac{\partial f_0}{\partial E_k}\right)}{I_0(E_k) + \frac{1}{\tau_m^{el}(E_k)}}$$

where $f_0(E_k)$ is the equilibrium Fermi-Dirac distribution function that is given by:

$$f_0(E_k) = \frac{1}{1+\exp\left(\frac{E-E_F}{k_BT}\right)} = \frac{1}{1+\exp\left(\frac{E-E_c+E_c-E_F}{k_BT}\right)} =$$

$$= \frac{1}{1+\exp\left(\frac{E_k+E_c-E_F}{k_BT}\right)}$$