(F) Rode's ITERATIVE PROCEDURE

- When the scattering process is inelastic and anisotropic, as it is the case for polar optical phonon scattering in GaAs, the RTA can not be used since it is impossible to define a simple relaxation time $\tau_f(E)$ that does not depend upon the distribution function. For this cases, the iterative technique due to Rode can be quite successful in calculating the actual distribution function under low-field conditions.

- To derive Rode's method, we start with the BTE for the case of steady-state conditions and no spatial gradients:

$$-\frac{e}{\hbar}\vec{\mathcal{E}}\cdot\nabla_k f = \sum_{\vec{k}'}\left\{S(\vec{k}',\vec{k})\,f(\vec{k}')[1-f(\vec{k})] - S(\vec{k},\vec{k}')\,f(\vec{k})[1-f(\vec{k}')]\right\}$$

$$= \sum_{\vec{k}'}\left\{S_{k',k}\,f'(1-f) - S_{k,k'}\,f(1-f')\right\}$$

If we use Legendre expansion for the distribution function and keep only terms that are linear in the field, we have:

$$f(k) = f_0(k) + g(k)\cos\theta + \underbrace{\mathcal{O}(\cos^2\theta)}_{\text{higher order terms}}$$

The LHS of the BTE becomes:

$$-\frac{e}{\hbar}\vec{\mathcal{E}}\cdot\nabla_k f = -e\,\vec{v}\cdot\vec{\mathcal{E}}\,\frac{\partial f_0}{\partial E} = -e v\mathcal{E}\cos\theta\left(\frac{\partial f_0}{\partial E}\right), \quad \theta = \measuredangle(\vec{v},\vec{\mathcal{E}})$$

or:

$$LHS = -e v\mathcal{E}\cos\theta\cdot\frac{\partial}{\partial E}\left[f_0 + g(k)\cos\theta\right]$$

$$= -e v\mathcal{E}\cos\theta\cdot\left[\frac{\partial f_0}{\partial E} + \underbrace{\cos\theta\,\frac{\partial g(k)}{\partial E}}_{\text{higher-order term}}\right] \approx -e v\mathcal{E}\cos\theta\,\frac{\partial f_0}{\partial E}$$

The collision term on the RHs becomes:

$$\frac{\partial f}{\partial t}\bigg|_{coll} = \sum_{\vec{k}'} \Big[S_{k',k} \left(f_0' + g'\cos\theta' \right) \left(1 - f_0 - g\cos\theta \right) - $$
$$ - S_{k,k'} \left(f_0 + g\cos\theta \right) \left(1 - f_0' - g'\cos\theta' \right) \Big]$$

$$\cong \sum_{\vec{k}'} \Big\{ S_{k',k} \left[f_0'(1-f_0) - \underline{f_0' g\cos\theta} + g'\underline{\underline{\cos}}\,\theta'(1-f_0) \right] - $$
$$ - S_{k,k'} \left[f_0(1-f_0') - f_0 \underline{\underline{g}}'\cos\theta' + \underline{g\cos}\,\theta(1-f_0') \right] \Big\}$$

$\uparrow$

ignored higher (second)order terms.

$$\frac{\partial f}{\partial t}\bigg|_{coll} = \sum_{\vec{k}'} \Big\{ g'\cos\theta' \left[S_{k',k}(1-f_0) + S_{k,k'} f_0 \right] - $$
$$ - g\cos\theta \left[f_0' S_{k',k} + S_{k,k'}(1-f_0') \right] + $$
$$ + \left[S_{k',k} f_0'(1-f_0) - S_{k,k'} f_0 (1-f_0') \right] \Big\}$$

0 by detailed balance

Hence: $$\frac{\partial f}{\partial t}\bigg|_{coll} = \sum_{\vec{k}'} \Big\{ g'\cos\theta' \left[S_{k',k}(1-f_0) + S_{k,k'} f_0 \right] - $$
$$ - g\cos\theta \left[f_0' S_{k',k} + S_{k,k'}(1-f_0') \right] \Big\}$$

- We now split the scattering processes into elastic and inelastic processes, i.e.

$$S_{k,k'} = S^{el}_{k,k'} + S^{in}_{k,k'}$$ and similarly for $S_{k',k}$.

→ For the elastic scattering processes, we have: $g(k') = g(k)$ i.e. $g = g'$, $f_0 = f_0'$ which gives:

$$\frac{\partial f}{\partial t}\bigg|^{el.}_{coll} = \sum_{k'} g(k) \Big\{ \left[S_{el}(k',k)(1-f_0) + S^{el}_{k,k'} f_0 \right] \cos\theta' - $$
$$ - \left[S^{el}_{k',k} f_0' + S^{el}_{k,k'}(1-f_0') \cos\theta \right\} = $$
$$ = \sum_{k'} g(k) \Big\{ S^{el}_{k',k} \left[(1-f_0)\cos\theta' - f_0\cos\theta \right] + S^{el}_{k,k'} \left[f_0\cos\theta' - (1-f_0)\cos\theta \right] \Big\}$$

The principle of detailed balance for elastic scattering gives: $S(\vec{k},\vec{k}') = S(\vec{k}',\vec{k})$ which should have been expected. Also noting that:

ignore since averages to zero

$$\frac{\cos\theta'}{\cos\theta} = tg\,\theta \sin\alpha \cancel{\sin\varphi} + \cos\alpha$$

we find:

$$\left.\frac{\partial f}{\partial t}\right|_{coll}^{el} = \sum_{\vec{k}'} g(\vec{k}) S_{K,K'}^{el} \cos\theta \left[(1-\cancel{f_0})\cos\alpha - \cancel{f_0} + \cancel{f_0\cos\alpha} - (1-\cancel{f_0})\right]$$

$$= -g(\vec{k})\cos\theta \sum_{\vec{k}'} S_{K,K'}^{el}(1-\cos\alpha) = -\frac{g(\vec{k})\cos\theta}{\tau_m^{el}(\vec{k})}$$

→ We now consider the inelastic part of the collision integral (the one that includes inelastic scattering processes):

$$\cos\theta\, S_0 = \left.\frac{\partial f}{\partial t}\right|_{coll}^{in} = \cos\theta \sum_{\vec{k}'} \Big\{ g(\vec{k}') \left[S_{k',k}^{in}(1-f_0) + S_{k,k'}^{in} f_0\right] \cos\alpha - g(\vec{k}) \left[f_0' S_{K',K}^{in} + S_{K,K'}^{in}(1-f_0')\right] \Big\}$$

i.e.

$$S_0 = \overbrace{\sum_{\vec{k}'} g(k') \cos\alpha \left[S_{k',k}^{in}(1-f_0) + S_{k,k'}^{in} f_0\right]}^{\tilde{I}}$$

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

to summarize, for inelastic scattering processes we have:

$$\left.\frac{\partial f}{\partial t}\right|_{coll}^{in} = \cos\theta \left\{\tilde{I}(\vec{k}) - g(\vec{k}) I_0(\vec{k})\right\}$$

where:

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

$$I_0(k) = \sum_{\vec{k}'} \left[S^{in}_{k',k} f_0(\vec{k}') + S^{in}_{k,k'}\left(1 - f_0(\vec{k}')\right) \right] \rightarrow \frac{1}{\tau(k)} \text{ for nondegenerate case}$$

- Combining all these results together, leads to:

$$-ev\varepsilon \cancel{\cos\theta}\left(\frac{\partial f_0}{\partial E}\right) = -\frac{g(k)\cancel{\cos\theta}}{\tau_m^{el}(k)} + \cancel{\cos\theta}\left[\tilde{I}(k) - g(k) I_0(k)\right]$$

$$= -g(k)\cancel{\cos\theta}\left[\frac{1}{\tau_m^{el}} + I_0(k)\right] + \cancel{\cos\theta}\,\tilde{I}(k)$$

or:

$$g(k)\left[\frac{1}{\tau_m^{el}} + I_0(k)\right] = ev\varepsilon\left(\frac{\partial f_0}{\partial E}\right) + \tilde{I}(k)$$

$$\boxed{g(k) = \frac{\tilde{I}(k) + ev\varepsilon\left(\frac{\partial f_0}{\partial E}\right)}{\frac{1}{\tau_m^{el}(k)} + I_0(k)}}$$

- Special cases: If the inelastic scattering process is isotropic, then $\tilde{I}(k) = 0$ and we have:

$$g(k) = \frac{ev\varepsilon\left(\frac{\partial f_0}{\partial E}\right)}{I_0(k) + \frac{1}{\tau_m^{el}(k)}} \rightarrow \text{Relaxation-time approximation result. No iterative procedure needed.}$$

- For a general case of inelastic and anisotropic scattering process, the procedure for calculating $g(k)$ or $g(E)$ is the following:

  (a) Set up a mesh in energy space from 0 to some large enough values

  (b) use as initial guess, for example $g^0(k) = 0$. This will give $\tilde{I}^{(0)}(k) = 0$ and:

$$g_{3}^{(1)}(k) = \frac{ev\mathcal{E}\left(\frac{\partial f_0}{\partial E}\right)}{I_0(k) + \frac{1}{\tau_m^{el}(k)}}$$

(c) The value for $g^{(1)}(k)$ is used in evaluating:

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

$$g^{(2)}(k) = \frac{\tilde{I}^{(1)}(k) + ev\mathcal{E}\left(\frac{\partial f_0}{\partial E}\right)}{I_0(k) + \frac{1}{\tau_m^{el}(k)}}$$

(d) Repeat procedure → step (c) until convergence is achieved.

(e) once convergence is achieved, calculate the carrier drift velocity, i.e. current using:

$$\vec{J} = -\frac{e}{V}\sum_k \vec{v} f(E) = -\frac{e}{V}\sum_k \vec{v}\, g(k)\cos\theta$$

Assuming $\vec{\mathcal{E}} = \mathcal{E}\vec{i_z}$, $v_z = v\cos\theta$ and

$$J_z = -\frac{e}{V}\sum_k v\cos^2\theta\, g(k) = -\frac{e}{\cancel{V}}\frac{\cancel{V}}{(2\pi)^3}\cdot 2\int_0^{2\pi} d\varphi \int_{-1}^{1} d(\cos\theta)\int_0^{\infty} k^2 dk\; v\cos^2\theta\, g(k)$$

$$= -\frac{2e}{(2\pi)^{\cancel{3}2}}\, \cancel{2\pi}\cdot\frac{2}{3}\int_0^{\infty} k^2 dk\; v\, g(k)$$

Using: $E = \hbar^2 k^2/2m^*$ we get: $dE = \frac{\hbar^2}{m^*} k\,dk$ and $k = \sqrt{\frac{2m^* E}{\hbar^2}}$

Hence: $v k^2 dk = \frac{\hbar k^2}{m^*} k\,dk = \frac{\cancel{\hbar}}{\cancel{m^*}}\,\frac{2\cancel{m^*}E}{\hbar^{\cancel{2}}}\cdot\frac{m^*}{\hbar^2}\,dE = \frac{m^* E}{\hbar^3}\,dE$.

This leads to:

$$J_z = -\frac{2e}{4\pi^2}\,\frac{2}{3}\,\frac{m^*}{\hbar^3}\int_0^{\infty} E\,g(E)\,dE = -\frac{4em^*}{12\pi^2\hbar^3}\int_0^{\infty} E\,g(E)\,dE = -\frac{em^*}{3\pi^2\hbar^3}\int_0^{\infty} E\,g(E)\,dE$$

Since: $J_z = +en\mu_n\mathcal{E}$, this finally leads to:

$$\cancel{+}\cancel{e}n\mu_n\varepsilon \overset{\ominus}{=} \cancel{+}\frac{\cancel{e}m^*}{3\pi^2\hbar^3}\int_0^\infty Eg(E)\,dE$$

and the low-field mobility equals to:

$$\boxed{\mu_n = -\frac{1}{n\varepsilon}\frac{m^*}{3\pi^2\hbar^3}\int_0^\infty Eg(E)\,dE}$$

Expressing the electron density in terms of the equilibrium distribution function leads to:

$$n = 2\frac{1}{(2\pi)^3}\,2\pi\cdot 2\int_0^\infty f_0k^2\,dk = \frac{1}{\pi^2}\int_0^\infty k\cdot k\,dk\,f_0 = \frac{1}{\pi^2}\int_0^\infty\sqrt{\frac{2m}{\hbar^2}}\sqrt{E}f_0\frac{m^*}{\hbar^2}\,dE$$

$$= \frac{1}{\pi^2}\sqrt{\frac{2m^*}{\hbar^2}}\,\frac{m^*}{\hbar^2}\int_0^\infty f_0E^{1/2}\,dE = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_0^\infty f_0E^{1/2}\,dE$$

The low-field mobility is then given by:

$$\mu_n = -\frac{\cancel{m^*}}{3\cancel{\pi^2}\cancel{\hbar^3}}\,\frac{\int_0^\infty E[g(E)/\varepsilon]\,dE}{\frac{1}{\cancel{2\pi^2}}\frac{\cancel{2m^*}\sqrt{2m^*}}{\cancel{\hbar^3}}\int_0^\infty f_0E^{1/2}\,dE} =$$

$$= \frac{-1}{3\sqrt{2m^*}}\cdot\frac{\int_0^\infty E[g(E)/\varepsilon]\,dE}{\int_0^\infty f_0E^{1/2}\,dE}$$

Check units:

$$[\mu] = \frac{1}{\sqrt{kg}}\,\frac{J\cdot\cancel{J}}{\frac{V}{m}\sqrt{J}\cdot\cancel{J}} = \frac{1}{\sqrt{kg}}\,\frac{m}{V}\sqrt{J} = \frac{1}{\sqrt{\cancel{kg}}}\,\frac{m}{V}\sqrt{\cancel{kg}\frac{m^2}{s^2}} = \frac{m^2}{V\cdot s}\ \text{(OK)}$$

Alternative derivation of Rode's method:

$$-\frac{e}{\hbar}\hbar\varepsilon v\cos\theta\,\frac{\partial f_T}{\partial E} = \sum_{k'}\left[S' f_T'(1-f_T) - S f_T(1-f_T')\right]$$

where the total distribution function is given by: $f_T = f_0 + g(k)\overset{x}{\widetilde{\cos\theta}}$, f_0 being the equilibrium part of the distribution and g being the perturbation part of the distribution function that is linear (to first order in the driving force). Then:

$$-\frac{e}{\hbar}\varepsilon v\hbar\cos\theta\left[\frac{\partial f_0}{\partial E} + \cos\theta\,\frac{\partial g}{\partial E}\right] = \sum_{k'} S'(f_0'+g'x')(1-f_0-g\cdot x) -$$
$$- S(f_0+gx)(1-f_0'-g'x')\Big]$$

$$= \sum_{k'}\Big\{S'\Big[f_0'(1-f_0) - \cancel{f_0'}\underline{gx} + \underline{\underline{\cancel{g'}x'}} - \cancel{f_0}\underline{\underline{g'}}x' - g'x'gx\Big] -$$
$$- S\Big[f_0(1-f_0') - \cancel{f_0}\underline{\underline{g'}}x' + \underline{gx} - \cancel{gx}f_0' - gxg'\underline{\underline{x'}}\Big]\Big\} \quad \text{where } x=\cos\theta,\ x'=\cos\theta'$$

From previous lecture we noted that $x' \to x\cos\alpha$. Using this gives:

$$-\frac{e}{\cancel{\hbar}}\cancel{\hbar} v\cos\theta\,\frac{\partial f_0}{\partial E} - \frac{e}{\cancel{\hbar}}\varepsilon\cancel{\hbar} v\cos^2\theta\,\frac{\partial g}{\partial E} =$$
$$= \sum_{k'}\Big\{S' f_0'(1-f_0) - [S(1-f_0') + S'f_0']gx + [S'(1-f_0) + Sf_0]g'x'$$
$$- Sf_0(1-f_0') + (S-S')gxg'x'\Big\}$$

$$\to \sum_{k'}\Big\{S' f_0'(1-f_0) - [S(1-f_0') + S'f_0']g\cos\theta + [S'(1-f_0) + Sf_0]g'\cos\alpha\cos\theta$$
$$- Sf_0(1-f_0') + (S-S')gg'\cos\alpha\cos^2\theta\Big\}$$

(a) Integrating against $d(\cos\theta)$ gives:

$$\underbrace{-e\varepsilon\cancel{v}\cdot\frac{2}{3}\,\frac{\partial g}{\partial E}}_{\substack{0\\ \text{second order in }\varepsilon}} = 2\sum_{k'}\left[S'f_0'(1-f_0) - Sf_0(1-f_0')\right] +$$
$$+ \frac{2}{3}\sum_{k'}\underbrace{(S-S')g\cancel{g}'\cos\alpha}_{\text{second-order in }\varepsilon}$$

(b) Multiplying by $\cos\theta$ and integrating against $d(\cos\theta)$ gives:

$$-ev\,\cancel{\tfrac{2}{3}}\,\frac{\partial f_0}{\partial E} = -\sum_{k'}\Big\{\left[S(1-f_0') + S'f_0'\right]g - \left[S'(1-f_0) + Sf_0\right]g'\cos\alpha\Big\}\cancel{\tfrac{2}{3}}$$
$$= -g\sum_{k'}\left[S(1-f_0') + S'f_0'\right] + \sum_{k'}\left[S'(1-f_0) + Sf_0\right]g'\cos\alpha$$

Therefore: $$-ev\frac{\partial f_0}{\partial E} = -g\sum_{k'}\left[S(1-f_0') + S'f_0'\right] + \sum_{k'}\left[S'(1-f_0) + Sf_0\right]g'\cos\alpha$$

We now split the scattering process into elastic and inelastic component. Also, from detailed balance we have $S_{el}' = S_{el}$ since $E' = E$ for elastic scattering. Then:

$$-ev\frac{\partial f_0}{\partial E} = -g\sum_{k'}\left\{1 - \cancel{f_0} + \cancel{f_0} - (1 - \cancel{f_0} + \cancel{f_0})\cos\alpha\right\}S_{el}(\vec{k},\vec{k}')$$

$$-g(k)\underbrace{\sum_{k'}\left[S_{in}(1-f_0') + S_{in}'f_0'\right]}_{I_0(k)} + \underbrace{\sum_{k'}\left[S_{in}'(1-f_0) + S_{in}f_0\right]g(k')\cos\alpha}_{\tilde{I}(k)}$$

$$-ev\frac{\partial f_0}{\partial E} = -g(k)\sum_{k'}(1-\cos\alpha)S_{el}(\vec{k},\vec{k}') - g(k)I_0(k) + \tilde{I}(k)$$

$$= -\frac{g(k)}{\tau_m^{el}(k)} - g(k)I_0(k) + \tilde{I}(k) = -\left[\frac{1}{\tau_m^{el}(k)} + I_0(k)\right]g(k) + \tilde{I}(k)$$

Solving this last expression with respect to $g(k)$ gives:

$$g(k) = \frac{-\tilde{I}(k) - ev\frac{\partial f_0}{\partial E}}{-\left[\frac{1}{\tau_m^{el}(k)} + I_0(k)\right]} = \boxed{\frac{\tilde{I}(k) + ev\frac{\partial f_0}{\partial E}}{\frac{1}{\tau_m^{el}(k)} + I_0(k)} = g(k)}$$

where: $$I_0(k) = \sum_{k'}\left\{S_{in}(\vec{k},\vec{k}')\left[1 - f_0(k')\right] + S_{in}(\vec{k}',\vec{k})f_0(\vec{k}')\right\} \xrightarrow[\text{nondegenerate limit}]{} \frac{1}{\tau_{in}(k)}$$

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

<u>Limits</u>: → elastic scattering only $\Rightarrow I_0(k) = \tilde{I}(k) = 0 \Rightarrow g(k) = \frac{ev\frac{\partial f_0}{\partial E}}{\frac{1}{\tau_m^{el}(k)}}$ (RTA)

→ isotropic scattering only $\Rightarrow \tilde{I}(k) = 0 \Rightarrow g(k) = \frac{ev\,\partial f_0/\partial E}{\frac{1}{\tau_m^{el}(k)} + I_0(k)}$ (RTA)

<u>conductivity</u>: $$J = -en\frac{\cancel{2}\int\frac{d^3k}{(2\pi)^3}v\cos\theta\, g(k)\cos\theta}{\cancel{2}\int\frac{d^3k}{(2\pi)^3}f_0(k)} = -en\frac{\cancel{2\pi}\cdot\frac{\cancel{2}}{3}\int_0^\infty k^2dk\; v g(k)}{\cancel{2\pi}\cdot\cancel{2}\int k^2dk\, f_0(k)}$$

$$J = -\cancel{n}e\,\frac{1}{3}\;\frac{\int_0^\infty k^2 dk\; v g(k)}{\int_0^\infty k^2 dk\, f_0(k)} = +\cancel{n}e\,\mu_n\,\varepsilon$$

Therefore, the low-field mobility is given by

$$\boxed{\mu_n = -\frac{1}{3}\;\frac{\int_0^\infty k^2 dk\;[v g(k)/\varepsilon]}{\int_0^\infty k^2 dk\; f_0(k)}}$$

$$= -\frac{1}{3}\;\frac{\int_0^\infty \cancel{\alpha}\sqrt{E}\,dE\,[v(E)\,g(E)/\varepsilon]}{\int_0^\infty \cancel{\alpha}\sqrt{E}\; f_0(E)\,dE}$$

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

Notes from Rode's paper:

(1) The rate of convergence of the iteration sequence $g(k)$ or $g(E)$ is exponential. Hence, the procedure requires very few iterations for any reasonable accuracy

(2) In the case of either elastic or isotropic scattering processes, one step is needed to get to the right answer, i.e. Rode's method immediately gives the relaxation-time approximation result.

(3) Also note from case (a), when the terms that are of second order in the electric field are kept, that elastic scattering affects the non-symmetric part of the distribution, whereas inelastic scattering affects the symmetric part of the distribution.