ECE-656: Fall 2009

Lecture 14: Solving the BTE: 1D / RTA

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

the BTE

$$f\left(\vec{r},\vec{p},t\right)$$

$$\frac{\partial f}{\partial t}+\vec{\upsilon}\bullet\nabla_r f+\vec{F}_e\bullet\nabla_p f=$$

$$\sum_{p'} S\left(\vec{p}',\vec{p}\right) f\left(\vec{p}'\right)\left[1-f\left(\vec{p}\right)\right]-\sum_{p'} S\left(\vec{p},\vec{p}'\right) f\left(\vec{p}\right)\left[1-f\left(\vec{p}'\right)\right]$$

Six-dimensional integro-differential equation for *f*(*r*, *p*, *t*).

outline

1) **The RTA**

2) Solving the BTE: drift

3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary

collision integral

$$\hat{C}f = \sum_{p'} S(\vec{p}\,', \vec{p}) f(\vec{p}\,')\left[1 - f(\vec{p})\right] - \sum_{p'} S(\vec{p}, \vec{p}\,') f(\vec{p})\left[1 - f(\vec{p}\,')\right]$$

non-degenerate…

$$\hat{C}f = \sum_{p'} S(\vec{p}\,', \vec{p}) f(\vec{p}\,') - \sum_{p'} S(\vec{p}, \vec{p}\,') f(\vec{p})$$

$$\hat{C}f = \sum_{p'} S(\vec{p}\,', \vec{p}) f(\vec{p}\,') - f(\vec{p}) \sum_{p'} S(\vec{p}, \vec{p}\,')$$

$$\hat{C}f = \sum_{p'} S(\vec{p}\,', \vec{p}) f(\vec{p}\,') - \frac{f(\vec{p})}{\tau}$$

"scattering rate"

$$\frac{1}{\tau} = \sum_{p'} S(\vec{p}, \vec{p}\,')$$

RTA

$$\hat{C}f = \sum_{p'} S(\vec{p}', \vec{p}) f(\vec{p}') - \frac{f(\vec{p})}{\tau}$$

$$\hat{C}f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_f}\right)$$

$$\hat{C}f = \frac{f_0(\vec{p})}{\tau_f} - \frac{f(\vec{p})}{\tau_f}$$

in-scattering – out-scattering

See Lundstrom: pp. 139-141. The RTA can be justified when the scattering is **isotropic and/or elastic** in which case the proper time to use is the “momentum relaxation time.”

RTA (ii)

$$f_0(\vec{p}) = \frac{1}{1 + e^{[E_C + E(\vec{p}) - E_F]/k_B T}} \approx e^{\frac{[E_F - E_C - E(\vec{p})]}{k_B T}}$$

$$f_0(\vec{p}) = f_0(-\vec{p})$$

even in momentum
"symmetric"

$$f_S(\vec{p}) = \frac{1}{1 + e^{[E_C + E(\vec{p}) - F_n]/k_B T}} \approx e^{\frac{[F_n - E_C - E(\vec{p})]}{k_B T}}$$

$$f(\vec{p}) = f_S(\vec{p}) + f_A(\vec{p})$$

$$f_A(\vec{p}) = -f_A(-\vec{p})$$

odd in momentum
"anti-symmetric"

$$\hat{C}f = -\left(\frac{f(\vec{p}) - f_S(\vec{p})}{\tau_f}\right) = -\frac{f_A(\vec{p})}{\tau_f}$$

RTA (iii)

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\left(\frac{f(\vec{p}) - f_0(\vec{p})}{\tau_f} \right) = -\frac{f_A(\vec{p})}{\tau_f}$$

assume:

$$\nabla_r f = 0 \qquad \vec{F}_e = -q\vec{\mathcal{E}} = 0$$

$$\frac{\partial f_A(\vec{p},t)}{\partial t} = -\frac{f_A(\vec{p},t)}{\tau_f}$$

$$f_A(\vec{p},t) = f_A(\vec{p},0)e^{-t/\tau_f}$$

Perturbations from equilibrium decay exponentially with time.

$$\left.\frac{\partial n(x,t)}{\partial t}\right|_{R-G} = -\frac{(n-n_0)}{\tau}$$

outline

1) The RTA

2) Solving the BTE: drift

3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary

BTE

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - q\mathcal{E}_x \frac{\partial f}{\partial(\hbar k_x)} = \hat{C} f$$

$$-q\mathcal{E}_x \frac{\partial f}{\partial p_x} = -\frac{(f - f_0)}{\tau_f}$$

steady-state, spatially homogeneous, RTA

$$-q\mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{(f - f_0)}{\tau_f}$$

$$f(\vec{p}) = f_0(\vec{p}) + q\,\tau_f\,\mathcal{E}_x \frac{\partial f_0}{\partial p_x}$$

solution

$$f(\vec{p}) = f_0(\vec{p}) + q\,\tau_f\,\mathcal{E}_x \frac{\partial f_0}{\partial p_x}$$

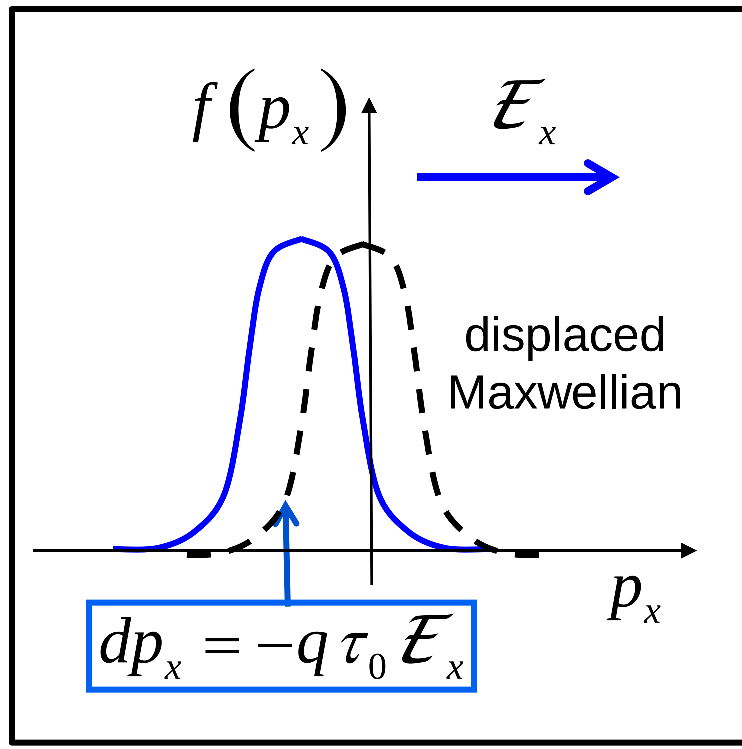
$$\tau_f(E) = \tau_0$$

Recall:

$$g(x+dx) \approx g(x) + \frac{\partial g}{\partial x} dx + \ldots$$

$$f(\vec{p}) = f_0(\vec{p} + dp_x \hat{x})$$

$$dp_x = q\,\tau_0\,\mathcal{E}_x$$



So the distribution has been displaced by p_d is a direction ***opposite*** to the electric field

current

$$\langle p_x \rangle = -q\,\tau_0\,\mathcal{E}_x$$

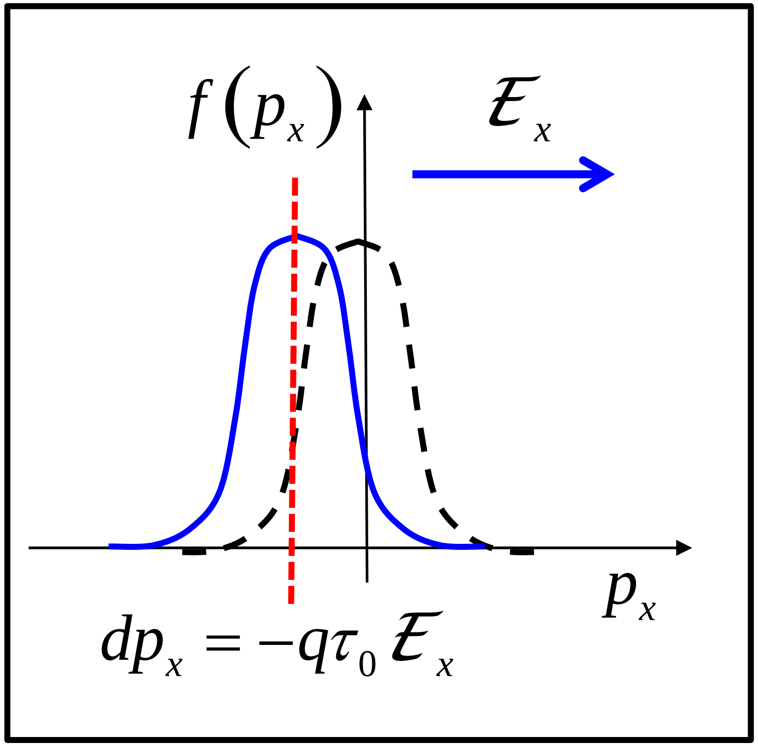
$$\langle \upsilon_x \rangle = \frac{\langle p_x \rangle}{m^*} = \frac{-q\,\tau_0}{m^*}\mathcal{E}_x = -\mu_n \mathcal{E}_x$$

$$\mu_n = \frac{q\,\tau_0}{m^*}$$

$$I = qn_L \langle \upsilon_x \rangle = n_L q \mu_n \mathcal{E}_x$$

$$I/W = qn_S \langle \upsilon_x \rangle = n_S q \mu_n \mathcal{E}_x$$

$$I/A = qn \langle \upsilon_x \rangle = nq \mu_n \mathcal{E}_x$$



alternative solution method

$$-q\mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{\left(f - f_0\right)}{\tau_f(E)}$$

$$f(\vec{p}) = f_0(\vec{p}) + q\tau\mathcal{E}_x \frac{\partial f_0}{\partial p_x} = f_0(\vec{p}) + q\tau_f\mathcal{E}_x \frac{\partial f_0}{\partial E}\frac{\partial E}{\partial p_x}$$

$$\Rightarrow$$

$$f(\vec{p}) = f_0(\vec{p}) - q\tau_f\mathcal{E}_x \frac{f_0}{k_B T}\upsilon_x$$

$$\Rightarrow$$

$$f_A(\vec{p}) = -\frac{q\tau_f\upsilon_x}{k_B T} f_0 \mathcal{E}_x$$

$$\Rightarrow$$

$$f_0(p) = e^{(E_F - E)/k_B T}$$

$$\frac{\partial f_0}{\partial E} = -\frac{1}{k_B T} f_0$$

$$\frac{\partial E}{\partial p_x} = \upsilon_x$$

alternative solution method (ii)

$$\langle \upsilon_x \rangle = \frac{\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x f(\vec{k})}{\frac{1}{\Omega}\sum_{\vec{k}} f(\vec{k})} = \frac{1}{n\Omega}\sum_{\vec{k}} \upsilon_x f_A(\vec{k}) \qquad f_A(\vec{p}) = -\frac{q\tau_f \upsilon_x}{k_B T} f_0 \mathcal{E}_x$$

$$\langle \upsilon_x \rangle = \frac{1}{n\Omega}\sum_{\vec{k}} \upsilon_x \left[-\frac{q\tau\upsilon_x}{k_B T} f_0 \mathcal{E}_x \right] = -\frac{q}{nk_B T}\left\{ \frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x^2 \tau(E) f_0 \right\}\mathcal{E}_x$$

$$\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x^2 \tau(E) f_0 = n\langle \upsilon_x^2 \tau_f \rangle$$

$$\langle \upsilon_x \rangle = -\frac{q\langle \upsilon_x^2 \tau_f \rangle}{k_B T}\mathcal{E}_x$$

alternative solution (iii)

$$\langle \upsilon_x \rangle = -\frac{q\langle \upsilon_x^2 \tau_f \rangle}{k_B T}\mathcal{E}_x$$

assume: $\tau_f(E) = \tau_0$

$$\langle \upsilon_x \rangle = -\frac{q\,\tau_0}{k_B T}\langle \upsilon_x^2 \rangle \mathcal{E}_x$$

$$\langle \upsilon_x \rangle = -\frac{q\,\tau_0}{m^*(k_B T/2)}\left(\frac{m^*\langle \upsilon_x^2 \rangle}{2}\right)\mathcal{E}_x$$

$$\left(\frac{m^*\langle \upsilon_x^2 \rangle}{2}\right) = \frac{k_B T}{2}$$

$$\langle \upsilon_x \rangle = -\left(\frac{q\,\tau_0}{m^*}\right)\mathcal{E}_x = -\mu_n \mathcal{E}_x$$

$$\mu_n = \frac{q\,\tau_0}{m^*}$$

outline

1) The RTA

2) Solving the BTE: drift

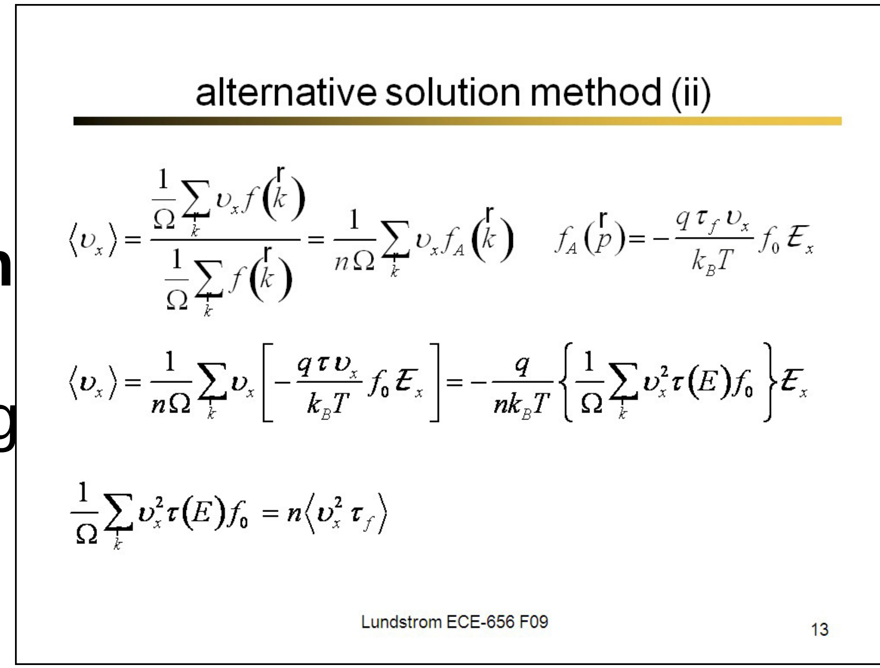
3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary



diffusion

$$\frac{\partial f}{\partial t} + \upsilon_x \frac{\partial f}{\partial x} - \frac{q\mathcal{E}_x}{\hbar} \frac{\partial f}{\partial k_x} = -\frac{(f - f_0)}{\tau_f}$$

steady-state, zero electric field

$$\upsilon_x \frac{\partial f}{\partial x} = -\frac{f_A}{\tau_f}$$

$$f_A = -\tau_f \, \upsilon_x \frac{\partial f_0}{\partial x}$$

$$\langle \upsilon_x \rangle = \frac{\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x f_A(\vec{k})}{\frac{1}{\Omega}\sum_{\vec{k}} f_0(\vec{k})} = -\frac{1}{n\Omega}\sum_{\vec{k}} \upsilon_x^2 \tau_f \frac{\partial f_0}{\partial x} = -\frac{1}{n}\frac{\partial}{\partial x}\left\{\frac{1}{\Omega}\sum_{\vec{k}} \upsilon_x^2 \tau_f \, f_0\right\}$$

diffusion

$$n\langle \upsilon_x \rangle = -\frac{\partial}{\partial x}\left\{\frac{1}{\Omega}\sum_k \upsilon_x^2 \tau_f \; f_0\right\}$$

$$n\langle \upsilon_x \rangle = -\frac{\partial}{\partial x}\left\{ n\langle \upsilon_x^2 \tau_f \rangle \right\} = -\langle \upsilon_x^2 \tau_f \rangle \frac{\partial n}{\partial x}$$

$$\langle \upsilon_x^2 \tau_f \rangle \equiv D_n = \left(\frac{k_B T}{q}\right)\frac{q\,\tau_0}{m^*}$$

$$\langle \upsilon_x \rangle == -D_n \frac{1}{n}\frac{\partial n}{\partial x}$$

$$D_n = \langle \upsilon_x^2 \tau_f \rangle \qquad \frac{D_n}{\mu_n} = \frac{k_B T}{q}$$

drift + diffusion

$$\langle \upsilon_x \rangle = -\mu_n \mathcal{E}_x \qquad \langle \upsilon_x \rangle == -D_n \frac{1}{n}\frac{\partial n}{\partial x}$$

$$J_{nx} = -nq\langle \upsilon_x \rangle = -nq\left(\langle \upsilon_x \rangle\big|_{drift} + \langle \upsilon_x \rangle\big|_{diff} \right)$$

$$J_{nx} = -nq\langle \upsilon_x \rangle = nq\mu_n E_x = qD_n\, dn/dx$$

$$D_n/\mu_n = k_B T/q$$

$$\mu_n = q\,\tau_0/m^*$$

But what if the scattering time is not constant?

outline

1) The RTA

2) Solving the BTE: drift

3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary

BTE solution

$$D_n = \langle \upsilon_x^2 \tau_f \rangle$$

$$\mu_n = \frac{D_n}{(k_B T/q)}$$

$$\langle \upsilon_x \rangle = -\mu_n \mathcal{E}_x$$

$$\mu_n = \frac{q\langle \upsilon_x^2 \tau_f \rangle}{k_B T} = \frac{q\langle \upsilon^2 \tau_f \rangle}{3k_B T}$$

$$\left(\upsilon^2 = \upsilon_x^2 + \upsilon_y^2 + \upsilon_z^2 \rightarrow \upsilon_x^2 = \upsilon^2/3\right)$$

$$\mu_n = \frac{q}{3k_B T} \frac{\langle \upsilon^2 \tau_f \rangle}{\langle \upsilon^2 \rangle} \langle \upsilon^2 \rangle$$

$$\mu_n = \frac{q}{3k_B T} \frac{\langle \upsilon^2 \tau_f \rangle}{\langle \upsilon^2 \rangle} \frac{2}{m^*} \left\langle \frac{1}{2} m^* \upsilon^2 \right\rangle$$

$$\mu_n = \frac{q}{m^*} \frac{\langle \upsilon^2 \tau_f \rangle}{\langle \upsilon^2 \rangle}$$

energy-dependent tau

$$\mu_n = \frac{q\langle\langle \tau_f \rangle\rangle}{m^*}$$

$$\langle\langle \tau_f \rangle\rangle \equiv \frac{\langle \upsilon^2 \tau_f \rangle}{\langle \upsilon^2 \rangle} = \frac{\langle E\tau_f(E)\rangle}{\langle E \rangle}$$

$$\langle X \rangle \equiv \frac{\sum_k X f_0(E)}{\sum_k f_0(E)}$$

$$\tau_f(E) = \tau_0 \left(E/k_B T\right)^s$$

"power law scattering"

$$\langle\langle \tau_f \rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

$$\langle\langle \tau_f \rangle\rangle \equiv \frac{\langle E\tau_f(E)\rangle}{\langle E \rangle}$$

Lundstrom, p. 137-138

energy-dependent tau

$$\mu_n = \frac{q\langle\langle\tau_f\rangle\rangle}{m^*}$$

$$\langle\langle\tau_f\rangle\rangle \equiv \frac{\langle E\tau_f(E)\rangle}{\langle E\rangle}$$

$$\tau_f(E) = \tau_0 \left(E/k_BT\right)^s$$

$$\langle\langle\tau_f\rangle\rangle = \tau_0 \frac{\Gamma(s+5/2)}{\Gamma(5/2)}$$

$$\Gamma(n) = (n-1)!$$

$$\Gamma(1/2) = \sqrt{\pi}$$

$$\Gamma(p+1) = p\Gamma(p)$$

s = -1/2: acoustic phonon scattering

s = +3/2 : ionized impurity scattering

outline

1) The RTA

2) Solving the BTE: drift

3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary

1D transport: BTE

$$f_A = -q\left(-\frac{\partial f_0}{\partial E}\right)\left(\upsilon_x \tau_f\right)\mathcal{E}_x$$

Consider a 1D nanowire with 1 subband occupied.

$$I_x = \frac{1}{L}\sum_{k_x}(-q)\upsilon_x f_A = \frac{1}{\pi}\int_{-\infty}^{+\infty}(-q)\upsilon_x f_A \, dk_x$$

$$dk_x \sqcap = \frac{1}{\hbar}\frac{d\left(\hbar k_x\right)}{dE} = \frac{\upsilon_x}{\hbar}$$

$$I_x = \left\{\frac{2q^2}{h}\int_0^{+\infty}\left(2\upsilon_x \tau_f\right)\left(-\frac{\partial f_0}{\partial E}\right)dE\right\}\mathcal{E}_x$$

$$I_x = \left\{\frac{2q^2}{h}\int_0^{+\infty}\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right\}\mathcal{E}_x$$

$$\lambda\left(E\right) = 2\upsilon_x \tau_f$$

BTE → Landauer

$$I_x = \left\{ \frac{2q^2}{h} \int_0^{+\infty} \frac{\lambda(E)}{L} \left(-\frac{\partial f_0}{\partial E} \right) dE \right\} \mathcal{E}_x L$$

$$I = -I_x = \left\{ \frac{2q^2}{h} \int_0^{+\infty} \frac{\lambda(E)}{L} \left(-\frac{\partial f_0}{\partial E} \right) dE \right\} V$$

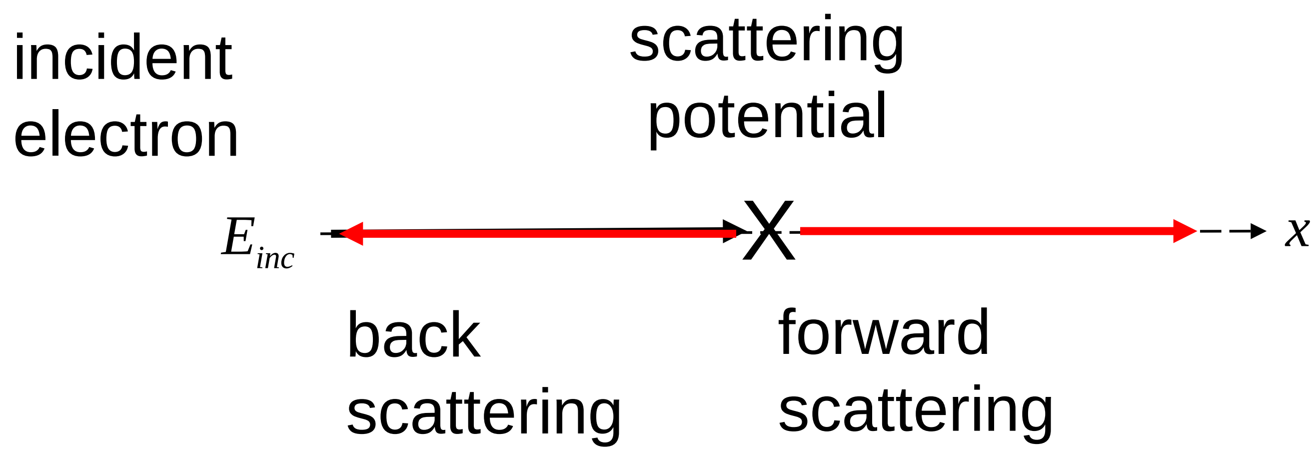
$$G = \frac{2q^2}{h} \int_0^{+\infty} T(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$T(E) = \frac{\lambda(E)}{L}$$

$$\lambda(E) = 2\upsilon_x \tau_f$$

So the BTE gives the same answer as the Landauer approach in the diffusive limie - **providing that we properly define the mfp.**

why does mfp = 2 v tau?



If we assume that the scattering is ***isotropic*** (equal probability of scattering forward or back) then average time between backscattering events is 2λ

$$\lambda(E) = 2\upsilon(E)\tau_f(E)$$

outline

1) The RTA

2) Solving the BTE: drift

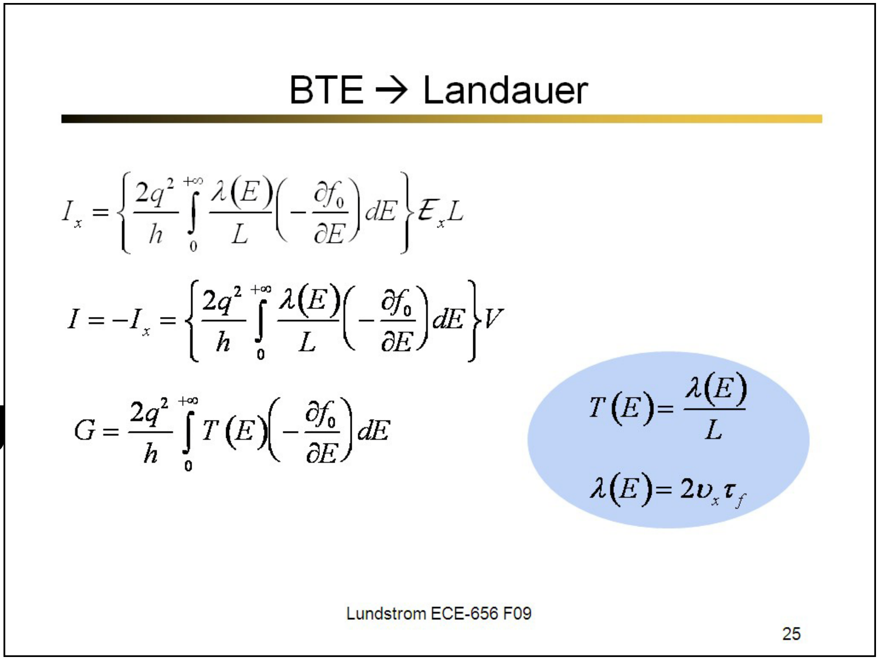
3) Solving the BTE: diffusion

4) Energy-dependent scattering time

5) Relation to Landauer

6) Discussion

7) Summary



BTE → Landauer

$$I_x = \left\{\frac{2q^2}{h}\int_0^{+\infty}\frac{\lambda(E)}{L}\left(-\frac{\partial f_0}{\partial E}\right)dE\right\}\mathcal{E}_x L$$

$$I = -I_x = \left\{\frac{2q^2}{h}\int_0^{+\infty}\frac{\lambda(E)}{L}\left(-\frac{\partial f_0}{\partial E}\right)dE\right\}V$$

$$G = \frac{2q^2}{h}\int_0^{+\infty}T(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$T(E) = \frac{\lambda(E)}{L}$$

$$\lambda(E) = 2\upsilon_x\tau_f$$

Lundstrom ECE-656 F09

25

multiple scattering mechanisms

$$\left.\frac{df}{dt}\right|_{coll} = -\frac{f_A}{\tau_f} \rightarrow \left.\frac{df}{dt}\right|_{coll} = -\frac{f_A}{\tau_1} - \frac{f_A}{\tau_2} = -\frac{f_A}{\tau_{tot}}$$

$$\frac{1}{\tau_{tot}} = \frac{1}{\tau_1} + \frac{1}{\tau_2}$$

$$\tau_1 = \tau_{10}\left(E/k_B T\right)^{s_1} \qquad \tau_2 = \tau_{20}\left(E/k_B T\right)^{s_2}$$

$$\tau_{tot} = \frac{\tau_{10}\tau_{20}\left(E/k_B T\right)^{s_1+s_2}}{\tau_{10}\left(E/k_B T\right)^{s_1} + \tau_{10}\left(E/k_B T\right)^{s_2}}$$

$$\neq \tau_0^{tot}\left(E/k_B T\right)^{s_{tot}}$$

$$\mu_n = \frac{q\langle\langle\tau_f\rangle\rangle}{m^*}$$

Mathiessen's rule

$$s_1 = s_2 = s \qquad \tau_{tot} = \frac{\tau_{10}\tau_{20}}{\tau_{10} + \tau_{10}}\left(E/k_BT\right)^s = \tau_0^{tot}\left(E/k_BT\right)^s$$

$$\mu_n = \frac{q\langle\langle\tau_f\rangle\rangle}{m^*}$$

$$\mu_{tot} = \frac{q\,\tau_0^{tot}}{m^*}\frac{\Gamma\left(s+5/2\right)}{\Gamma\left(5/2\right)}$$

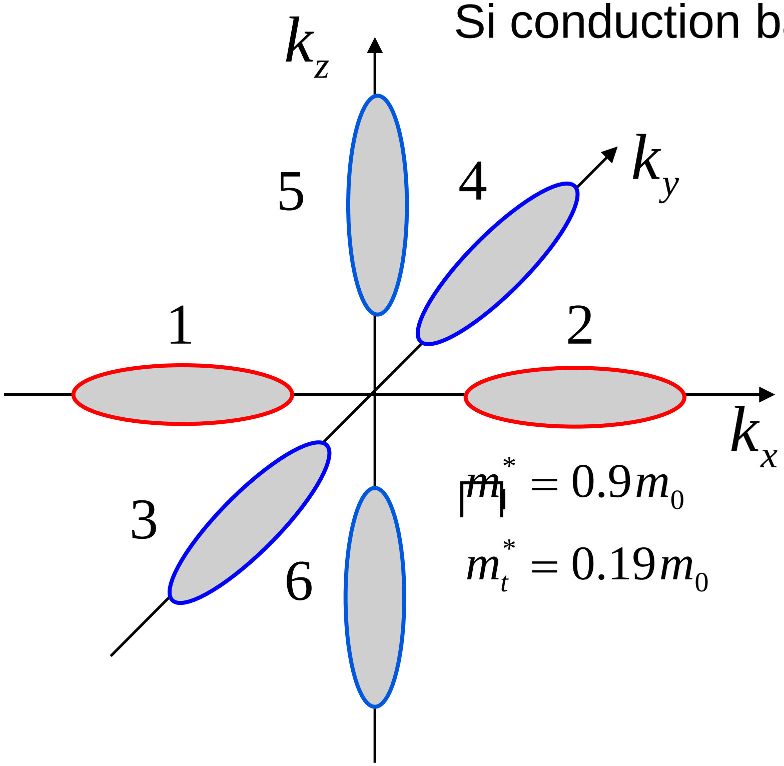
$$\frac{1}{\mu_{tot}} = \frac{1}{\mu_1} + \frac{1}{\mu_2}$$

Mathiessen's Rule

$$\frac{1}{\tau_{tot}\left(E\right)} = \frac{1}{\tau_1\left(E\right)} + \frac{1}{\tau_2\left(E\right)}$$

ellipsoidal bands

Si conduction band



$$m_l^* = 0.9 m_0$$

$$m_t^* = 0.19 m_0$$

$$\sigma_{1,2} = \frac{n}{6} q \frac{q\langle\langle\tau\rangle\rangle}{m_l^*}$$

$$\sigma_{3-6} = \frac{n}{6} q \frac{q\langle\langle\tau\rangle\rangle}{m_t^*}$$

$$\sigma = 2\sigma_1 + 4\sigma_3$$

$$\sigma_{1,2} = \frac{n}{6} q \left[\frac{1}{3m_l^*} + \frac{2}{3m_t^*}\right] q\langle\langle\tau\rangle\rangle$$

$$\frac{1}{m_c^*} = \frac{1}{3m_l^*} + \frac{2}{3m_t^*}$$

"conductivity effective mass"

questions

1) The RTA
2) Solving the BTE: drift
3) Solving the BTE: diffusion
4) Energy-dependent scattering time
5) Relation to Landauer
6) Discussion
7) Summary