ECE 656: Electronic Transport in Semiconductors Fall 2017

# The Collision Integral

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# BTE

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

$$\left.\frac{\partial f}{\partial t}\right)_{coll} = \hat{C} f = \text{in-scattering - out-scattering}$$

"collision operator" or "collision integral"

# Outline

1) **Collision integral (operator**)
2) Equilibrium
3) Relaxation Time Approximation

# Collision integral (or operator)

(in-scattering) - (out-scattering)

$$\hat{C}f\left(\vec{r},\vec{p},t\right)=\sum_{p'}S\left(\vec{p}'\to\vec{p}\right)f\left(\vec{p}'\right)\left[1-f\left(\vec{p}\right)\right]-\sum_{p'}S\left(\vec{p}\to\vec{p}'\right)f\left(\vec{p}\right)\left[1-f\left(\vec{p}'\right)\right]$$

probability that the state at p' is occupied

probability that the state at p is empty

# Nondegenerate collision integral

$$\hat{C}f\left(\vec{r},\vec{p},t\right)=\sum_{p'}S\left(\vec{p}'\to\vec{p}\right)f\left(\vec{p}'\right)-\sum_{p'}S\left(\vec{p}\to\vec{p}'\right)f\left(\vec{p}\right)$$

probability that the state at p’ is occupied

probability that the state at p is empty = 1

$$\hat{C}f\left(\vec{r},\vec{p},t\right)=\sum_{p'}S\left(\vec{p}'\to\vec{p}\right)f\left(\vec{p}'\right)-\frac{f\left(\vec{p}\right)}{\tau\left(\vec{p}\right)}$$

in-scattering is the hard part.

# Outline

1) Collision integral (or operator)
2) **Equilibrium**
3) Relaxation Time Approximation

# Collision integral in equilibrium

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

in equilibrium: $\hat{C}f = 0$ $\quad f(\vec{p}) = f_0(E)$ $\quad f(\vec{p}') = f_0(E')$

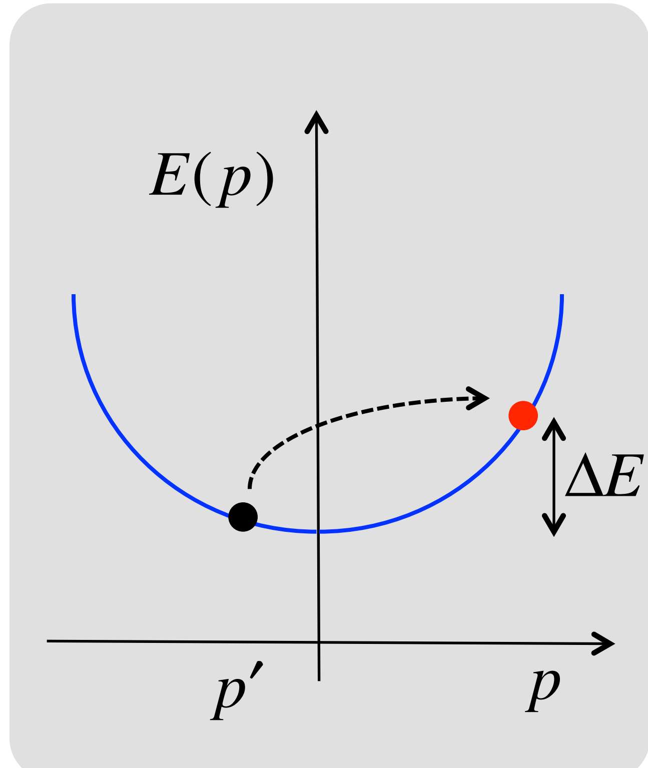
**and** the principle of detailed balance holds.

$$S(\vec{p}' \to \vec{p}) f_0(E') \left[1 - f_0(E)\right] - S(\vec{p} \to \vec{p}') f_0(E) \left[1 - f_0(E')\right] = 0$$

**no sum over other states.**

# Collision integral

$$\frac{S(\vec{p}\,' \rightarrow \vec{p})}{S(\vec{p} \rightarrow \vec{p}\,')} = e^{-\Delta E / k_B T} \qquad \Delta E = E(p) - E(p')$$




1) elastic scattering:

$$S(\vec{p} \rightarrow \vec{p}\,') = S(\vec{p}\,' \rightarrow \vec{p})$$

2) phonon scattering:

$$\frac{S^{ABS}(\vec{p}\,' \rightarrow \vec{p})}{S^{EMS}(\vec{p} \rightarrow \vec{p}\,')} = e^{-\hbar\omega / k_B T} = \frac{N_\omega}{N_\omega + 1}$$

# Outline

1) Collision integral (or operator)
2) Equilibrium
3) **Relaxation Time Approximation**

# Collision integral

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

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

See Lundstrom (FCT): 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."

# Symmetric and anti-symmetric components

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

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

even in momentum
"symmetric"

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

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

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

odd in momentum
"anti-symmetric"

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

# Physical meaning

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

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.

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

(a familiar example)

# RTA

$$\hat{C}f\left(\vec{r},\vec{p},t\right)=\sum_{p'}S\left(\vec{p}'\rightarrow\vec{p}\right)f\left(\vec{p}'\right)\left[1-f\left(\vec{p}\right)\right]-\sum_{p'}S\left(\vec{p}\rightarrow\vec{p}'\right)f\left(\vec{p}\right)\left[1-f\left(\vec{p}'\right)\right]$$

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

$$\delta f=f\left(\vec{p}\right)-f_S\left(\vec{p}\right)$$

# RTA

The (microscopic) momentum relaxation time is valid near-equilibrium and:

1) For isotropic scattering with MB statistics

or

2) For elastic scattering.

When valid, the characteristic time is the momentum relaxation time.

See Lundstrom, FCT, Chapter 3, pp. 139-141 for more discussion.

# Questions?

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

$$\frac{\partial f}{\partial t} + \vec{\upsilon} \bullet \nabla_r f + \vec{F}_e \bullet \nabla_p f = -\left( \frac{f - f_S}{\tau_m} \right)$$