Week6 – Carrier Transport

ECE 695-O Semiconductor Transport Theory

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Instructor: Byoung-Don Kong

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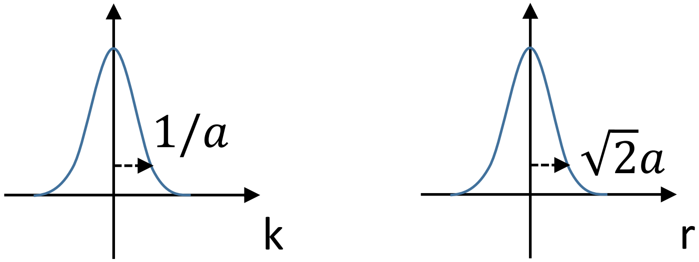
- Boltzmann Transport Equation

Wave Packet Representation

- We can represent the solution of Schrödinger Eq. in wave packet form (i.e. Gaussian wave packet).



- By choosing these boundaries properly, we can satisfy Pauli's exclusion principle with the minimum uncertainty. ($\Delta x \Delta p > \hbar/2$)
- The wave packet picture also satisfies the classical eq. of motions if we take the average of the values.

For example) $\langle \mathbf{v} \rangle = \frac{d\langle \mathbf{x} \rangle}{dt}$

- When the wave packet broadening is smaller than the dimension of our interest, we can treat it with the classical eq. of motions.

Boltzmann Transport Equation

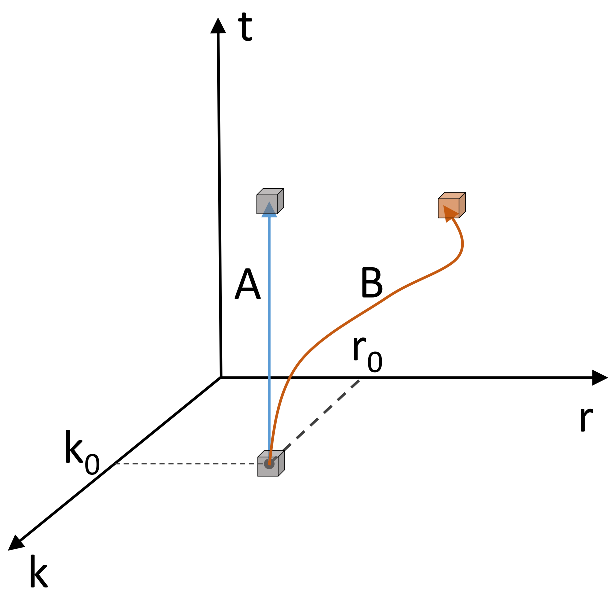
- Instead of chasing individual carriers whose numbers may easily go above the number of stars in our galaxy (~2.5 ± 1.5 x 10^{11}), dealing with the statistical character of a system of whole carriers is more advantageous (and practical).
- Thus, we will discuss about the time evolution of probability of occupation and distribution function.

❖ $f(\mathbf{k}, \mathbf{r}, t)$: probability distribution function.

- In equilibrium, carrier distribution can be described by

$f(\mathbf{k}, \mathbf{r}, t) = f_0(\mathcal{E})$: Fermi Dirac Distribution.

Boltzmann Transport Equation(2)



Phase space

Each state evolve following the equation of motions: $\hbar \frac{d\mathbf{k}}{dt} = q\mathbf{E}$

$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}$$

- If we assume a trajectory such as A, there is no evolution of states. In this case, we only need to count in-and-out of the states to see the change in f. This is partial time derivative.
- When each state evolves such as the trajectory B, we need to trace the evolution of states and count in-and-out from states. This is total time derivative.
- When there is no path-cross (meaning the occupation probability of the box does not change), $\frac{df}{dt} = 0$.
- This is not true because we ignored some facts such as momentum altering events (i.e. scattering) or generation-recombination.

Boltzmann Transport Equation(3)

- By including scattering and generation-recombination(g-r).

$$\frac{df}{dt} = \left.\frac{\partial f}{\partial t}\right)_{scatt.} + \left.\frac{\partial f}{\partial t}\right)_{g-r} \qquad (1)$$

- On the other hand, the total derivative of distribution function can be separated like:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \underbrace{\boxed{\frac{d\mathbf{k}}{dt}}}_{=\frac{\mathbf{F}}{\hbar}} \cdot \nabla_{\mathbf{k}} f + \underbrace{\boxed{\frac{d\mathbf{r}}{dt}}}_{=\mathbf{v}} \cdot \nabla_{\mathbf{r}} f \qquad (2)$$

- Then, the equation becomes (by putting an equal sign between right sides of (1) and (2))

$$\frac{\partial f}{\partial t} = \underbrace{-\frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f}_{\text{diffusion term}} \underbrace{- \mathbf{v} \cdot \nabla_{\mathbf{r}} f}_{\text{drift term}} + \left.\frac{\partial f}{\partial t}\right)_{scatt.} + \left.\frac{\partial f}{\partial t}\right)_{g-r}$$

Boltzmann Transport Equation(4)

- We can assume Lorentz force acting on the charged particles

$$\mathbf{F} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \qquad\qquad e = \pm q$$

- As for the velocity, we know that

$$\mathbf{v} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}$$

- Then, the equation becomes

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E} \cdot \nabla_{\mathbf{r}} f - \frac{e}{\hbar} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{k}} f + \left.\frac{\partial f}{\partial t}\right)_{scatt.} + \left.\frac{\partial f}{\partial t}\right)_{g-r}$$

- Now, we need to figure out $\left.\frac{\partial f}{\partial t}\right)_{scatt.}$ and $\left.\frac{\partial f}{\partial t}\right)_{g-r}$.

Boltzmann Transport Equation(5)

- Scattering term ($\left.\frac{\partial f}{\partial t}\right)_{scatt.}$)
- A carrier scatter in or scatter out of a state.
  - Scattering in corresponds to gaining probability.
  - Scattering out corresponds to losing probability.
- Define $P_{\mathbf{kk}'}$ as the transitional probability for a particle to scatter from $\mathbf{k}$ to $\mathbf{k}'$. Then, the scattering probability is

$$P_{\mathbf{kk}'}\, f(\mathbf{k}, \mathbf{r}, t)[1 - f(\mathbf{k}', \mathbf{r}, t)]$$

fundamental strength of scattering

probability that a particle exist at $(\mathbf{k}, \mathbf{r}, t)$
(since there is no scattering if there is no particle)

probability that there is an empty slot at $(\mathbf{k}', \mathbf{r}, t)$
(since scattering cannot happen if there is no slot to go)

Boltzmann Transport Equation(6)

$$\Rightarrow \left.\frac{\partial f}{\partial t}\right)_{scatt.} = -\int P_{\mathbf{kk}'}\, f(\mathbf{k},\mathbf{r},t)[1-f(\mathbf{k}',\mathbf{r},t)]\frac{d^3k'}{8\pi^3}$$

$\mathbf{k} \rightarrow \mathbf{k}'$:negative sign since the particle scatters out from $\mathbf{k}$

- V disappears since we will consider this for unit volume
- It is $8\pi^3$, not $4\pi^3$ since spin degeneracy is not accounted here. (spin state does not change but it depends on the scattering mechanisms)

$$+\int P_{\mathbf{k}'\mathbf{k}}\, f(\mathbf{k}',\mathbf{r},t)[1-f(\mathbf{k},\mathbf{r},t)]\frac{d^3k'}{8\pi^3}$$

$\mathbf{k}' \rightarrow \mathbf{k}$:positive sign since the particle scatters into $\mathbf{k}$

Integration with respect to $\mathbf{k}'$

We can ignore $\left.\frac{\partial f}{\partial t}\right)_{g-r}$ term for the time being since in semiconductor g-r event is rare due to the band gap.

Boltzmann Transport Equation(7)

- Then, Boltzmann transport equation becomes

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\cdot\nabla_{\mathbf{r}}f - \frac{e}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}f$$
$$-\int\{P_{\mathbf{k}\mathbf{k}'}\,f(\mathbf{k},\mathbf{r},t)[1-f(\mathbf{k}',\mathbf{r},t)]$$
$$-P_{\mathbf{k}'\mathbf{k}}\,f(\mathbf{k}',\mathbf{r},t)[1-f(\mathbf{k},\mathbf{r},t)]\}\frac{d^3k'}{8\pi^3} \quad \cancel{+\left.\frac{\partial f}{\partial t}\right)_{g-r}}$$

- We will seek for a solution of BTE in the case of small deviation from the equilibrium state. (under adiabatic assumption)
- In equilibrium, $\frac{df}{dt} = \left.\frac{\partial f}{\partial t}\right)_{scatt.} + \left.\frac{\partial f}{\partial t}\right)_{g-r} = 0$, and since we assumed $\left.\frac{\partial f}{\partial t}\right)_{g-r} = 0$, $\left.\frac{\partial f}{\partial t}\right)_{scatt.}$ is also zero.
- In addition, $f(\mathbf{k},\mathbf{r},t) = f_0(\mathcal{E})$ that is Fermi-Dirac distribution.

(pay attention to the fact that right hand variable is energy)

Boltzmann Transport Equation(8)

- Then,

$$\left.\frac{\partial f}{\partial t}\right)_{scatt.} = \int \{P_{\mathbf{k}'\mathbf{k}}\, f(\mathbf{k}',\mathbf{r},t)[1-f(\mathbf{k},\mathbf{r},t)] - P_{\mathbf{k}\mathbf{k}'}\, f(\mathbf{k},\mathbf{r},t)[1-f(\mathbf{k}',\mathbf{r},t)]\}\frac{d^3k'}{8\pi^3} = 0$$

$$\Rightarrow P_{\mathbf{k}\mathbf{k}'}\, f_0(\mathcal{E})[1-f_0(\mathcal{E}')] = P_{\mathbf{k}'\mathbf{k}} f_0(\mathcal{E}')[1-f_0(\mathcal{E})]$$

$$\Rightarrow P_{\mathbf{k}'\mathbf{k}} = P_{\mathbf{k}\mathbf{k}'}\frac{f_0(\mathcal{E})[1-f_0(\mathcal{E}')]}{f_0(\mathcal{E}')[1-f_0(\mathcal{E})]}$$

(we will use this relation even in non-equilibrium cases though.)

- Plugging this into the equation back:

$$\left.\frac{\partial f}{\partial t}\right)_{scatt.} = \int P_{\mathbf{k}\mathbf{k}'}\frac{\{N\}}{f_0(\mathcal{E}')[1-f_0(\mathcal{E})]}\frac{d^3k'}{8\pi^3}$$

where $\{N\} = f_0(\mathcal{E})[1-f_0(\mathcal{E}')]f(\mathbf{k}',\mathbf{r},t)[1-f(\mathbf{k},\mathbf{r},t)] - f_0(\mathcal{E}')[1-f_0(\mathcal{E})]f(\mathbf{k},\mathbf{r},t)[1-f(\mathbf{k}',\mathbf{r},t)]$

Boltzmann Transport Equation(9)

- We can consider a small perturbation F such that

$$f(\mathbf{k},\mathbf{r},t) = f_0(\mathcal{E}) + F(\mathbf{k},\mathbf{r},t) .$$

- Then,

$$\{N\} = f_0(\mathcal{E})[1 - f_0(\mathcal{E}')]f(\mathbf{k}',\mathbf{r},t)[1 - f(\mathbf{k},\mathbf{r},t)] - f_0(\mathcal{E}')[1 - f_0(\mathcal{E})]f(\mathbf{k},\mathbf{r},t)[1 - f(\mathbf{k}',\mathbf{r},t)]$$

$$= F(\mathbf{k}',\mathbf{r},t)f_0(\mathcal{E})[1 - f_0(\mathcal{E}')] - F(\mathbf{k},\mathbf{r},t)f_0(\mathcal{E}')[1 - f_0(\mathcal{E})]$$

$$\cancel{+F(\mathbf{k}',\mathbf{r},t)F(\mathbf{k},\mathbf{r},t)[f_0(\mathcal{E}') - f_0(\mathcal{E})]} + \cdots$$

We ignore 2nd order or higher terms since F is a small deviation.

- We define F as

$$F(\mathbf{k},\mathbf{r},t) = -\underbrace{\phi(\mathbf{k},\mathbf{r},t)}\frac{\partial f_0}{\partial \mathcal{E}}$$

This is something like the first term when we expand $f(\mathbf{k},\mathbf{r},t)$ with respect to $f_0(\mathcal{E})$, i.e. $f(\mathbf{k},\mathbf{r},t) = f_0(\mathcal{E}) + \phi\frac{\partial f_0}{\partial \mathcal{E}} + \cdots$.
It is unknown and we need to find what it is.

Boltzmann Transport Equation(10)

- Since

$$f_0(\mathcal{E}) = \frac{1}{1 + e^{\mathcal{E}-\mu/_{k_B T}}}.$$

- Then,

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

- Replace $F(\mathbf{k}, \mathbf{r}, t)$ in $\{N\}$ with this

$$\begin{aligned}
\{N\} &= F(\mathbf{k}', \mathbf{r}, t) f_0(\mathcal{E})[1 - f_0(\mathcal{E}')] - F(\mathbf{k}, \mathbf{r}, t) f_0(\mathcal{E}')[1 - f_0(\mathcal{E})] \\
&= \frac{1}{k_B T} \phi(\mathbf{k}', \mathbf{r}, t) f_0(\mathcal{E}')[1 - f_0(\mathcal{E})] f_0(\mathcal{E})[1 - f_0(\mathcal{E}')] \\
&\quad - \frac{1}{k_B T} \phi(\mathbf{k}, \mathbf{r}, t) f_0(\mathcal{E})[1 - f_0(\mathcal{E}')] f_0(\mathcal{E}')[1 - f_0(\mathcal{E})] \\
&= \frac{f_0(\mathcal{E})[1 - f_0(\mathcal{E}')] f_0(\mathcal{E}')[1 - f_0(\mathcal{E})]}{k_B T} [\phi(\mathbf{k}', \mathbf{r}, t) - \phi(\mathbf{k}, \mathbf{r}, t)]
\end{aligned}$$

- Then,

$$\left.\frac{\partial f}{\partial t}\right)_{scatt.} = \int P_{\mathbf{k}\mathbf{k}'} \frac{\{N\}}{f_0(\mathcal{E}')[1 - f_0(\mathcal{E})]} \frac{d^3k'}{8\pi^3}$$

$$= \int P_{\mathbf{k}\mathbf{k}'} \frac{f_0(\mathcal{E})[1 - f_0(\mathcal{E}')]}{k_B T} [\phi(\mathbf{k}', \mathbf{r}, t) - \phi(\mathbf{k}, \mathbf{r}, t)] \frac{d^3k'}{8\pi^3}$$

Boltzmann Transport Equation(11)

- The Boltzmann transport equation then becomes

$$\frac{\partial f}{\partial t} = -\frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\cdot\nabla_{\mathbf{r}}f - \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f$$
$$+\frac{1}{k_B T}\frac{1}{8\pi^3}\int d^3k' P_{\mathbf{kk}'} f_0(\mathcal{E})[1 - f_0(\mathcal{E}')]\,[\phi(\mathbf{k}',\mathbf{r},t) - \phi(\mathbf{k},\mathbf{r},t)]$$

- In equilibrium, the time dependence and spatial dependence of T can be eliminated.
- $\frac{\partial f}{\partial t} = 0$ in steady state. In equilibrium $\frac{df}{dt} = 0$.
- However, in steady state, T is spatial function ($T(\mathbf{r})$).
- In steady state, $f_0(\mathcal{E})$ and $f_0(\mathcal{E}')$ have spatial dependence, too. ($f_0(\mathcal{E},\mathbf{r})$ and $f_0(\mathcal{E}',\mathbf{r})$).
- In this case, we can assume $\mathcal{E}_F$ varies slowly (which works like a local equilibrium).