# F. Results in Sections D and E rederived

Aim: Derive $\sigma$ again starting from Eq. (30) in a more straight forward way

Eq. (30): $f(\vec{k}) = f^0(\vec{k}) - \frac{e}{kT}\tau(\vec{k}) f^0(1-f^0)\,\vec{v}(\vec{k})\cdot\vec{\mathcal{E}}$

good $\vec{\mathcal{E}} = \mathcal{E}\hat{z}$, what we really want to get is some averaged drift velocity $\overline{v_z}$ (in direction of $\vec{\mathcal{E}}$), then $J = (-e)n\overline{v_z} \propto \mathcal{E}$

$\therefore$ Let's emphasize more on the velocity $v$ (rather than $\vec{k}$ or $\vec{p}$)

$$f(\vec{v}) = f_0(v) - \frac{e}{kT}\tau(v) f^0(1-f^0)\,\vec{v}\cdot\vec{\mathcal{E}} \qquad (30)$$

$$= \underbrace{f_0(v)}_{\text{isotropic}} - \frac{e}{kT}\tau(v)\underbrace{v\cos\theta}_{v_z\ (\because\ \parallel\ \vec{\mathcal{E}})} f^0(1-f^0)\,\mathcal{E} \qquad (30a)$$

$f(\vec{v})$ is the out-of-equilibrium distribution from which we want to evaluate $\overline{v_z}$

$$\therefore \boxed{\overline{v_z} = \frac{\int v_z\, f(\vec{v})\, d^3v}{\int f(\vec{v})\, d^3v}} \qquad (38)$$

with $f(\vec{v})$ given by Eq. (30a)

assumed to depend on $v = |v|$

**Denominator:**

$$\int f(\vec{v}) d^3v = \int \left[ f^0(v) - \frac{\tau(v)\, v\overbrace{\cos\theta}}{kT} \underbrace{f_0}_{\substack{f_0(\mathcal{E}) \\ \text{thus } f_0(v)}} (1-f_0)\, e\mathcal{E} \right] v^2 \underbrace{\sin\theta}\, dv\, \overbrace{d\theta}^{\int_0^\pi} \overbrace{d\phi}^{\int_0^{2\pi}}$$

$$\downarrow$$

$$= \int f^0(v) d^3v \qquad \underbrace{\qquad\qquad\qquad\qquad}_{\sim \int_0^\pi \cos\theta \sin\theta\, d\theta = 0}$$

$$\therefore \overline{v_z} = \underbrace{\frac{\int v_z f^0(v) d^3v}{\int f^0(v) d^3v}}_{1^{st} \text{ term} = 0} - \frac{e\mathcal{E}}{kT} \frac{\int \tau(v)\, \overbrace{v^2\cos^2\theta}^{v_z \cdot v_z}\, f_0 (1-f_0)\, v^2 \sin\theta\, dv\, d\theta\, d\phi}{\int f^0(v)\, v^2 \sin\theta\, dv\, d\theta\, d\phi}$$

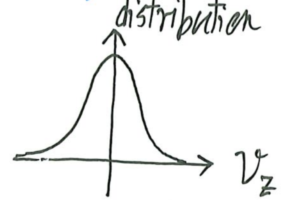
$1^{st}$ term $= 0$ $\quad \because \quad \dfrac{\int v_z f^0(v)\, d^3v}{\int f^0(v)\, d^3v}$ = "$v_z$" averaged over equilibrium distribution $f^0$

($f^0 = f^0(\varepsilon) = f^0(v)$ ← isotropic)

Example: Classical distribution

$$f^0(v) = \underbrace{A}_{\text{constant (e.g. } e^{-E_F/kT} \text{ with proper normalization factor)}} e^{-\varepsilon/kT}$$

$$= A\, \underbrace{e^{-\frac{1}{2}m^*(v_x^2+v_y^2+v_z^2)/kT}}_{} \sim e^{-\frac{1}{2}\frac{m^* v^2}{kT}}$$




$\underbrace{\text{equal chance to take on a value } +v_z \text{ and } -v_z}_{}$

$(\overline{v_z})_{\text{equil } f^0} = 0$ (no $\vec{J}$ at equilibrium)

But argument works as long as $f^0(\varepsilon)$ only

$\underbrace{\text{long as } f^0(\varepsilon)}_{\text{not necessarily } e^{-\frac{1}{2}m^* v^2/kT}}$

$$\therefore \overline{v_z} = -\frac{e\mathcal{E}}{kT} \frac{\int \tau(v)\, v^2 f_0 (1-f_0)\, v^2 \cos^2\theta \sin\theta \, dv\, d\theta\, d\phi}{\int f_0(v)\, v^2 \sin\theta\, dv\, d\theta\, d\phi}$$

[ integrands "function of $v$", integrating over $\theta$ and $\phi$ can be done]

$$= -\frac{e\mathcal{E}}{kT} \frac{\int_0^\infty \tau(v)\, v^2 f_0 \cdot (1-f_0)\, v^2 dv \cdot \frac{4\pi}{3}}{\int_0^\infty f_0(v)\, v^2 dv \cdot 4\pi}$$

$$= -\frac{e\mathcal{E}}{3kT} \underbrace{\frac{\int_0^\infty \tau(v)\, v^2 f_0 \cdot (1-f_0)\, v^2 dv}{\int_0^\infty f_0(v)\, v^2 dv}}_{\text{started to see the special average } \bar{\tau} \text{ as in Eq. (36)}} \qquad (39)$$

(General, good for metals, semiconductors)

$$= -\frac{e\mathcal{E}}{m^*}\bar{\tau} \qquad (\text{defines } \bar{\tau})$$

[this form will give $\sigma = \frac{ne^2}{m^*}\bar{\tau}$ and $\mu = \frac{e\bar{\tau}}{m^*}$]

So, $$\overline{\tau} = \frac{m^*}{3kT} \frac{\int_0^\infty \tau(v)\, v^2 f_0 \cdot (1-f_0)\, v^2 dv}{\int_0^\infty f_0(v)\, v^2 dv} \qquad (40) \qquad \left[\begin{array}{c}\text{still general}\\ \tau = \tau(v)\end{array}\right]$$

- At this point, let's restrict ourselves to <u>semiconductors</u> where

$$f_0 \cdot (1-f_0) \approx f_0 = A\, e^{-\varepsilon/kT} = A\, e^{-\frac{m^* v^2}{2kT}} \quad \text{(Boltzmann)}$$

$$\overline{\tau} = \frac{m^*}{3kT} \left[ \frac{\int \tau(v)\, v^2\, f_0(v)\, v^2 dv}{\int f_0(v)\, v^2 dv} \right] \equiv \frac{m^*}{3kT} \langle \tau(v)\, v^2 \rangle_0$$

where $\langle \tau(v) v^2 \rangle_0$ is average of "$\tau(v) v^2$" over the equilibrium $f^0(v)$

- For such a non-degenerate gas: $\frac{1}{2} m^* \langle v^2 \rangle_0 = \frac{3}{2} kT \Rightarrow \underbrace{\frac{m^*}{3kT}}_{\text{the prefactor}} = \frac{1}{\langle v^2 \rangle_0}$

$$\boxed{\therefore\ \overline{\tau} = \frac{\langle \tau(v) v^2 \rangle_0}{\langle v^2 \rangle_0}} \qquad (41)$$

① a non-trivial type of average from transport theory ...

② with a combination of averages involving the equilibrium $f^0(v)$ (linear response)

Read ① then ②

Making connection with Eq. (36)

$$\overline{\tau} = \frac{m^*}{3kT} \frac{\int \tau(v) \cdot v^2 f_0(v) v^2 dv}{\int f_0(v) v^2 dv}$$

$\because (\varepsilon - E_c) = \frac{1}{2} m^* v^2$

$\hookrightarrow d\varepsilon = m^* v dv$

$$= \underbrace{\frac{2}{3kT}} \left[ \frac{\int \tau(\varepsilon) (\varepsilon - E_c)^{3/2} \cdot f_0(\varepsilon) d\varepsilon}{\int (\varepsilon - E_c)^{1/2} f_0(\varepsilon) d\varepsilon} \right] = \underbrace{\frac{2}{m^* \langle v^2 \rangle_0}} \cdot \left[ \frac{\int \tau(\varepsilon) (\varepsilon - E_c)^{3/2} f_0(\varepsilon) d\varepsilon}{\int (\varepsilon - E_c)^{1/2} f_0(\varepsilon) d\varepsilon} \right]$$

But
$$\langle v^2 \rangle_0 = \frac{\int v^4 f_0(v) dv}{\int v^2 f_0(v) dv} = \frac{\int v^3 f_0(v) v dv}{\int v f_0(v) v dv} = \frac{\left(\frac{2}{m^*}\right)^{3/2} \int_{E_c}^{\infty} (\varepsilon - E_c)^{3/2} f_0(\varepsilon) d\varepsilon}{\left(\frac{2}{m^*}\right)^{1/2} \int_{E_c}^{\infty} (\varepsilon - E_c)^{1/2} f_0(\varepsilon) d\varepsilon}$$

$$\therefore \overline{\tau} = \frac{\int_{E_c}^{\infty} \tau(\varepsilon) (\varepsilon - E_c)^{3/2} f_0(\varepsilon) d\varepsilon}{\int_{E_c}^{\infty} (\varepsilon - E_c)^{3/2} f_0(\varepsilon) d\varepsilon}$$

(as in Eq. (36)!) $= \dfrac{\langle (\varepsilon - E_c) \tau(\varepsilon) \rangle_0}{\langle (\varepsilon - E_c) \rangle_0}$

- Empricially, $\tau(\varepsilon)$ for many scattering processes behaves as

$$\tau(\varepsilon) = \underset{\substack{\uparrow \\ \text{some constant time}}}{\tau_0} \left(\frac{\varepsilon}{kT}\right)^{s} \leftarrow \text{some power}$$

(e.g. from QM calculations)

Then

$$\bar{\tau} = \frac{\langle \tau(v)\, v^2 \rangle_0}{\langle v^2 \rangle_0} = \tau_0 \frac{\int_0^\infty \left(\frac{m^* v}{2kT}\right)^s e^{-\frac{m^* v^2}{2kT}} v^4\, dv}{\int_0^\infty e^{-\frac{m^* v^2}{2kT}} v^4\, dv} = \tau_0 \frac{\overbrace{\Gamma\left(s+\frac{5}{2}\right)}^{\text{effect of the average}}}{\underset{\substack{\uparrow \\ \text{Gamma function}}}{\Gamma}\left(\frac{5}{2}\right)}$$

Key Points

- Technique here is applicable to many different stimulation-response problems

$f = f^0 + \delta f$, then $\overline{v_z}$ and response

## G. Drift Velocity is much less than average thermal velocity

- $\delta f$ to 1st order in $\vec{\mathcal{E}}$ $\Rightarrow$ $f = f^0 + \underbrace{\delta f}$

a tiny shift leads to a drift velocity

particles are moving ($kT$), only that no net contribution to $J$

$$\boxed{\text{Consistency requires drift velocity} \ll \text{thermal velocity}}$$

Semiconductors: $n \sim 10^{15}\ \text{cm}^{-3} \sim 10^{21}\ \text{m}^{-3}$ (metals: $n \sim 10^{23}\ \text{cm}^{-3} \sim 10^{29}\ \text{m}^{-3}$)

$\bar{\tau} \sim 10^{-12}\ \text{s}$ (metals: $\bar{\tau} \sim 10^{-13}\ \text{s}$)

Consider $\mathcal{E} = 1\ \text{V/m} = 0.01\ \text{V/cm}$

$$|\bar{v}_z| = \frac{e\bar{\tau}}{m}\mathcal{E} = \frac{(1.6\times10^{-19})(10^{-12})}{9.1\times10^{-31}}\cdot(1) = 0.176\ \text{ms}^{-1} = 17.6\ \text{cm s}^{-1}$$

just take bare mass (for simplicity)

$$J = ne\overline{v_z} = 10^{21}\cdot(1.6\times10^{-19})\cdot(0.176) \sim 28.2 \text{ Ampere } m^{-2} \sim 0.00282 \text{ ampere } cm^{-2}$$

$$\sigma = \frac{J}{\mathcal{E}} = 28.2\ \Omega^{-1} m^{-1}\ ;\ \rho = \frac{1}{\sigma} = 3.55\ \Omega\text{-cm}$$ (c.f. metals $\sim \mu\Omega$-cm or $10^{-6}\ \Omega$-cm)

Since $\mathcal{E} = 1\ V/m$, $\mu = 0.176\ \dfrac{m s^{-1}}{V/m} = 0.176\ \underline{m^2} V^{-1} s^{-1} = 1760\ cm^2 V^{-1} s^{-1}$

Electrons in Semiconductors form a classical gas (Maxwell distribution of speeds)

$$\frac{1}{2} m \langle v^2 \rangle = \frac{3}{2} kT \Rightarrow \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3kT}{m}} = \underbrace{v_{rms}}_{\text{representative thermal velocity}}$$

$$v_{rms} = \sqrt{\frac{3kT}{m}} = \sqrt{\frac{3\times \overbrace{(0.025)}^{\frac{1}{40}eV}(1.6\times10^{-19})}{9.11\times10^{-19}}} \sim 115{,}000\ \underline{ms^{-1}} \sim 1.15\times\underline{10^7}\ \underline{cms^{-1}}$$

$$v_{rms} \gg |\overline{v_z}|$$ by a big margin!

even higher $\mathcal{E}$-field, with $m_e^*$, etc., approach is $\underline{\text{Valid}}$.

## H. Diffusion : A by-product

current density

c.f. charge/(area·time) = J

[ Outline of key ideas/results ]

- Driving force : $(-\underbrace{\vec{\nabla} n(\vec{r})}_{\text{concentration gradient}})$

from concentrated side diffuse to less condensated side ⇒ flux → #/(area·time) ← number current density

$$\vec{\Phi}_{diff} = -D\,\vec{\nabla} n$$

Let's consider for simplicity $n(z)$ and thus $-\frac{\partial n}{\partial z}$ only (gradient in $\hat{z}$-direction),

$$\boxed{\Phi_{diff} = -D\,\frac{\partial n}{\partial z}} \quad (42) \text{ Fick's law}^{+}$$

diffusion constant (a response function)

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$^{+}$ If we account for the charge of particles, then we get $J_{diff}$ (diffusion current density)

[In EM, continuity equation $\vec{\nabla}\cdot\vec{J} + \frac{\partial \rho}{\partial t} = 0$ if no generation or destruction of charges in small volume under consideration]

Similarly,

$$\underbrace{D \frac{\partial^2 n}{\partial z^2} = \frac{\partial n}{\partial t}}_{\text{Diffusion equation}^{+}} \quad (43)$$ if no particle generation/destruction

## Application of Boltzmann Transport Equation

Let's consider situations in which the classical Maxwell-Boltzmann distribution prevails at equilibrium.

- Practically, can set up $\frac{\partial n}{\partial z}$ readily in semiconductors (p-n junction), but not so in metals.

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+ Same form for heat flow equation. Even the time-dependent Schrödinger Equation has the "form" of a diffusive equation.

Focus only on diffusion (not considering the charges, only "particles")

Steady state

$$0 = -\vec{v}\cdot\vec{\nabla}_r f - \cancel{\frac{\vec{F}_{ext}}{\hbar}}^{\,0}\cdot\vec{\nabla}_k f + \left(\frac{-(f-f^0)}{\tau}\right)$$

$\underbrace{\vec{\nabla}_r f}_{n(z)}$ — will pick up $\frac{\partial n}{\partial z}$

$\underbrace{\frac{\vec{F}_{ext}}{\hbar}\cdot\vec{\nabla}_k f}$ (no $\vec{\mathcal{E}}_0$, no $\vec{B}$)

$$\therefore \quad 0 = -v_z\frac{\partial f}{\partial z} - \frac{(f-f^0)}{\tau(v)} \Rightarrow \underset{\text{unknown}}{f} = f^0 - v_z\,\tau(v)\underset{\text{unknown}}{\frac{\partial f}{\partial z}}$$

$$f = f^0 - v_z\,\tau(v)\frac{\partial f}{\partial z} \qquad (44)$$

$f^0$: no effect (no concentration gradient)

$\underbrace{- v_z\,\tau(v)\frac{\partial f}{\partial z}}$: want linear response effect that can be cast into a term with $f^0$

Next, extract the driving force

- Formally, the problem of having $n(z)$ is a problem of having a spatially-dependent $\mu(\vec{r})$ [or $E_F(\vec{r})$], so we could then pick up $\left(\frac{\partial \mu}{\partial z}\right)$ which is related to $\left(\frac{\partial n}{\partial z}\right)$

The end result is $f = f^{\circ} - v_z \tau(v) \frac{1}{n} \frac{\partial n}{\partial z} f^{\circ}$ (details omitted here)

Then $$\overline{v_z} = -\frac{1}{n}\frac{\partial n}{\partial z} \frac{\int \tau(v) \overbrace{v^2 \cos^2\theta}^{v_z \cdot v_z} f^{\circ}(v)\, v^2 \sin\theta \, dv\, d\theta\, d\phi}{\int f^{\circ}(v)\, v^2 \sin\theta\, dv\, d\theta\, d\phi}$$ (see p. XI-(55))

$$\Phi_{diffusion} = n\,\overline{v_z} = -\frac{1}{3}\frac{\partial n}{\partial z}\left[\frac{\int \tau(v)\, v^2 f^{\circ}(v)\, v^2 dv}{\int f^{\circ}(v)\, v^2 dv}\right]$$ (angular integrations done (c.f. Eq. 139))

$$= -\frac{1}{3}\frac{\partial n}{\partial z}\langle \tau(v)\, v^2 \rangle_0 \qquad (45)$$ (same $\langle \tau(v) v^2 \rangle_0$ in $\bar{\tau}$)

Recall: $\bar{\tau} = \dfrac{m^*}{3kT}\langle \tau(v)\, v^2 \rangle_0$ ; $\sigma = ne\mu_e = \dfrac{ne^2\bar{\tau}}{m^*} = ne\left(\dfrac{e}{m^*}\bar{\tau}\right)$

$$\Phi_{\text{diffusion}} = -\frac{1}{3}\frac{\partial n}{\partial z}\cdot\frac{3kT}{m^*}\bar{\tau} = -D\,\frac{\partial n}{\partial z}$$

(same $\bar{\tau}$ as in $\sigma$ and $\mu$)

$$\therefore\; D = \frac{kT}{m^*}\bar{\tau} \qquad (46)$$

(Physics: Scatterings work to relax system to equilibrium when driving forces are turned off)

$$= \frac{kT}{e}\,\frac{e}{m^*}\bar{\tau}$$

$$\Rightarrow \boxed{D = \frac{kT}{e}\cdot\mu} \qquad (47)$$

Diffusion constant (diffusive)

mobility (drift)

related!

Einstein Relation

$\tau$ dropped out of the relation!

[doesn't depend on how $\tau(v)$ behaves!]

True also for holes ($D_p$, $\mu_p$)

## Another by-product

(a) $$\Phi_{diffusion} = -\left(\frac{\partial n}{\partial z}\right)\cdot \underbrace{\frac{1}{3}\cdot\langle\tau(v)\,v^2\rangle_0}_{D} \quad\Rightarrow\quad D = \frac{1}{3}\langle\tau(v)v^2\rangle_0 \qquad (48)$$

but $v\cdot\tau(v) = \ell(v) =$ mean free path, then $D = \frac{1}{3}\langle v\,\ell\rangle_0$ (49)

- Special cases: if $\ell$ is independent of $v$, then $\tau(v) = \frac{\ell}{v} \Rightarrow v^2\tau(v) = \ell v$

$$D = \frac{1}{3}\,\ell\,\langle v\rangle_0$$

(b) Earlier, we used the expression

$$K = \frac{1}{3}\; c\cdot v\cdot \ell$$ for the thermal conductivity of insulator (due to phonons)

$c$: phonon specific heat; $v$: phonon velocity (sound); $\ell$: mean free path

now we see the origin (need to set up Boltzmann Transport Equation for $n(\vec{r},\vec{q},t)$, phonon distribution function)

- C is involved because it is the energy current density that matters and the driving force is $\left(-\vec{\nabla}T \text{ or } -\frac{\partial T}{\partial z}\right)$
- $n^{\circ} = \dfrac{1}{e^{\frac{\hbar\omega}{kT}} - 1}$ , but now $T = T(\vec{r})$ and so need to solve for $n(\vec{r}, \vec{q}) - n^{\circ} = \delta n$ by relaxation time approximation
- $K = \frac{1}{3} \cdot c \cdot v \cdot \ell$ (crude understanding)

$K$: measurable ✓

$c$: measurable ✓

$v$: sound speed ✓

$\ell$: $\underbrace{\text{hard to measure}}$

$\ell$ in semiconductors was found to be just $\underbrace{\text{tens of Å}}_{\text{too short!}}$ for phonons

($\because$ actually very specific average is involved) (deeper understanding)

Up to here, we discussed

- Drift (due to $\vec{\mathcal{E}}$) $\vec{J}_{drift}$
- Diffusion (due to $-\frac{\partial n}{\partial z}$ (OR $-\vec{\nabla} n(\vec{r})$)) $\underbrace{\text{for charged particles}}_{\vec{J}_{diffusive}}$ (electrons and holes)

The two concepts come into play in setting up the equilibrium situation in a p-n junction

- electrons (holes) from n-side (p-side) diffuse to p-side (n-side)
- remaining immobile +ve donors (-ve acceptors) on n-side (p-side) set up an electric field $\vec{\mathcal{E}}$, which counteracts the diffusive current