
Derivation of the Drift-Diffusion Equation

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Drift-Diffusion Equation - Applicability

Basic equations governing transport in semiconductors and semiconductor devices:

- **Instances where Drift-Diffusion Equation cannot be used**
 - Accelerations during rapidly changing electric fields (transient effects)
 - Non quasi-steady state
 - Non-Maxwellian distribution
 - Accurate prediction of the distribution or spread of the transport behavior is required
- **Instances when Drift-Diffusion Equation can represent the trend (or predict the mean behavior of the transport properties)**
 - Feature length of the semiconductors smaller than the mean free path of the carriers
- **Instances when Drift-Diffusion equations are accurate**
 - Quasi-steady state assumption holds (no transient effects)
 - Device feature lengths much greater than the mean free paths of the carrier

The Method of Moments

In the Method of Moments, both sides of a equation are multiplied by a function (a moment generating function) raised to a integer power, and then integrated over all space

$$\therefore A(x, k, t) + B(x, k, t) = C(x, k, t)$$

Multiplying by the Moment
generating Function $\Theta^n(k)$
(n = order of the moment)

$$\int \Theta^k(k) A(x, k, t) d^3k + \int \Theta^k(k) B(x, k, t) d^3k = \int \Theta^k(k) C(x, k, t) d^3k$$

Method of Moments Applied to the Boltzmann Transport Equation

The Boltzmann Transport Equation with relaxation time approximation:

$$\frac{\partial f}{\partial t} + \frac{\vec{F}_{ext}}{\hbar} \cdot \vec{\nabla}_k f + \vec{v} \cdot \vec{\nabla}_x f = -\frac{f - f_0}{\tau}$$

f = a classical distribution function at nonequilibrium state that represents the probability of finding a particle at position x , with momentum k and at time t . The subscript 0 corresponds to the equilibrium state

Multiplying throughout by the moment generating function Θ^n and integrating over all k space

$$\int \Theta^n \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \Theta^n (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \Theta^n (\vec{v} \cdot \vec{\nabla}_x f) d^3k = -\int \Theta^n \frac{f - f_0}{\tau} d^3k$$

Method of Moments Applied to the Boltzmann Transport Equation

If $\Theta = 1$ and $n = 1$ then:

$$\int \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \frac{f - f_0}{\tau} d^3k$$

↓ Simplifies to

$$\frac{\partial n}{\partial t} + \vec{\nabla}_x \cdot (n\vec{v}) = 0 \rightarrow \text{Carrier Continuity Equation}$$

If $\Theta = v$ and $n = 1$ then:

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$

↓ Simplifies to

$$J_n = nq\mu_n \vec{F} + qD_n \vec{\nabla}_x n \rightarrow \text{Drift-Diffusion Equation}$$

In the subsequent slides we would derive the Drift-Diffusion Equation from Boltzmann Transport Equation by utilizing this Method of Moments

Drift-Diffusion Equation Derivation – 1st. Term

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$

Velocity is time independent

$$\frac{\partial}{\partial t} \int \vec{v} f d^3k$$

$$n = \text{carrier concentration} = \int G(k) f(k) d^3k$$

$G(k) = \text{Density of states}$

$$= \frac{1}{V} \frac{dN}{dk} = \frac{2}{(2\pi)^3} = \frac{1}{4\pi^3}$$

$$\therefore n = \int \frac{1}{4\pi^3} f(k) d^3k = \int f'(k) d^3k$$

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k = \frac{\partial}{\partial t} (n\vec{v})$$

Drift-Diffusion Equation Derivation – 2nd. Term

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$

Identity: $\vec{F} \cdot \vec{\nabla} g = \vec{\nabla} \cdot (g\vec{F}) - g\vec{\nabla} \cdot \vec{F}$

$$\frac{1}{\hbar} \int \vec{v} (\vec{\nabla}_k \cdot f\vec{F}_{ext}) d^3k - \frac{1}{\hbar} \int f\vec{v} (\vec{\nabla}_k \cdot \vec{F}_{ext}) d^3k$$

Identity: $(g\vec{F} \cdot \vec{\nabla})\vec{G} = \vec{\nabla} \cdot (g\vec{F}\vec{G}) - \vec{G}\vec{\nabla} \cdot (g\vec{F})$

$$\frac{1}{\hbar} \left\{ \int [\vec{\nabla}_k (f\vec{v}\vec{F}_{ext}) - (f\vec{F}_{ext} \cdot \vec{\nabla}_k)\vec{v}] d^3k \right\}$$

f is finite and so the surface integral (integral of divergence of $f\vec{v}\vec{F}_{ext}$) at infinity vanishes identically

$$- \frac{1}{\hbar} \int (f\vec{F}_{ext} \cdot \vec{\nabla}_k)\vec{v} d^3k$$

Drift-Diffusion Equation Derivation – 2nd. Term (Continued)

Substituting:

$$-\frac{1}{\hbar} \int (f \vec{F}_{ext} \cdot \vec{\nabla}_k) \vec{v} d^3k - \frac{1}{\hbar} \int f \vec{v} (\vec{\nabla}_k \cdot \vec{F}_{ext}) d^3k$$

Substituting $-\vec{\nabla}_x E = \vec{F}_{ext}$

$$\frac{1}{\hbar} \int (f \vec{\nabla}_x E \cdot \vec{\nabla}_k) \vec{v} d^3k + \frac{1}{\hbar} \int f \vec{v} (\vec{\nabla}_k \cdot \vec{\nabla}_x E) d^3k$$

$$\vec{\nabla}_k \cdot \vec{\nabla}_x E = \vec{\nabla}_x \cdot \vec{\nabla}_k E = \hbar \vec{\nabla}_x \cdot \vec{v}$$

$$\int f \vec{v} (\vec{\nabla}_x \cdot \vec{v}) d^3k$$

Substituting, the second term is finally reduced to:

$$\frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k = \frac{1}{\hbar} \int (f \vec{\nabla}_x E \cdot \vec{\nabla}_k) \vec{v} d^3k + \int f \vec{v} (\vec{\nabla}_x \cdot \vec{v}) d^3k$$

Drift-Diffusion Equation Derivation – 3rd. Term

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$

Identity: $\vec{F} \cdot \vec{\nabla} g = \vec{\nabla} \cdot (g\vec{F}) - g\vec{\nabla} \cdot \vec{F}$

$$\int \vec{v} \vec{\nabla}_x \cdot (f\vec{v}) d^3k - \int \vec{v} f (\vec{\nabla}_x \cdot \vec{v}) d^3k$$

Identity: $\vec{G} \vec{\nabla} \cdot (g\vec{F}) = \vec{\nabla} \cdot (g\vec{F}\vec{G}) - (g\vec{F} \cdot \vec{\nabla})\vec{G}$

$$\int \vec{\nabla}_x \cdot (f\vec{v}\vec{v}) d^3k - \int (f\vec{v} \cdot \vec{\nabla}_x) \vec{v} d^3k$$

Substituting, the third term is finally reduced to:

$$\int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = \int \vec{\nabla}_x \cdot (f\vec{v}\vec{v}) d^3k - \int (f\vec{v} \cdot \vec{\nabla}_x) \vec{v} d^3k - \int \vec{v} f (\vec{\nabla}_x \cdot \vec{v}) d^3k$$

Drift-Diffusion Equation Derivation – Right Hand Term

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$

$$- \frac{1}{\tau} \int \vec{v} (f - f_0) d^3k$$

Recall $\int f d^3k = n$ and $\int \vec{v} f d^3k = \bar{v} n$

n = carrier concentration
 \bar{v} = average velocity

$$- n \frac{\bar{v} - \bar{v}_0}{\tau}$$

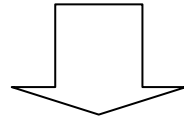
At equilibrium the ensemble velocity \bar{v}_0 (by definition) = 0

Substituting, the right hand term is finally reduced to:

$$- \int \vec{v} \frac{f - f_0}{\tau} d^3k = - n \frac{\bar{v}}{\tau}$$

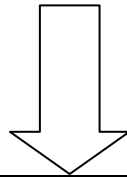
Drift-Diffusion Equation Derivation – General Form

$$\int \vec{v} \frac{\partial f}{\partial t} d^3k + \frac{1}{\hbar} \int \vec{v} (\vec{F}_{ext} \cdot \vec{\nabla}_k f) d^3k + \int \vec{v} (\vec{v} \cdot \vec{\nabla}_x f) d^3k = - \int \vec{v} \frac{f - f_0}{\tau} d^3k$$



$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\vec{\nabla}_x E \cdot \vec{\nabla}_k) \vec{v} d^3k + \int f\vec{v} (\vec{\nabla}_x \cdot \vec{v}) d^3k +$$

$$\int \vec{\nabla}_x \cdot (f\vec{v}\vec{v}) d^3k - \int (f\vec{v} \cdot \vec{\nabla}_x) \vec{v} d^3k - \int \vec{v} f (\vec{\nabla}_x \cdot \vec{v}) d^3k = -n \frac{\bar{v}}{\tau}$$



$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\vec{\nabla}_x E \cdot \vec{\nabla}_k) \vec{v} d^3k + \int \vec{\nabla}_x \cdot (f\vec{v}\vec{v}) d^3k - \int (f\vec{v} \cdot \vec{\nabla}_x) \vec{v} d^3k = -n \frac{\bar{v}}{\tau}$$

Standard Drift-Diffusion Equation for Electrons/Holes

The general Drift-Diffusion derived in the previous slides may be further simplified with the help of certain assumptions

- **Assumptions**

- The energy of the carriers, $E = \frac{\hbar^2 k^2}{2m}$

- Mass is isotropic and constant

$$\therefore E_x = E_y = E_z = E_i = \frac{1}{2} m v_i^2$$

- Material is isotropic, and so the spatial temperature gradient is zero

$$\vec{\nabla}_x E_i = 0$$

Standard Drift-Diffusion Equation for Electrons/Holes-Text Version

$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\bar{\nabla}_x E \cdot \bar{\nabla}_k) \bar{v} d^3k + \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k - \int (f\bar{v} \cdot \bar{\nabla}_x) \bar{v} d^3k = -n \frac{\bar{v}}{\tau}$$

Substituting $-\bar{\nabla}_x E = \bar{F}_{ext}$

$$-\frac{1}{\hbar} \int f\bar{F}_{ext} \cdot \bar{\nabla}_k \bar{v} d^3k$$

$$\left. \begin{aligned} E = \frac{\hbar^2 k^2}{2m} &\Rightarrow \bar{\nabla}_k E = \frac{\hbar^2 \bar{k}}{m} \xrightarrow{\bar{k}=m\bar{v}} \bar{v} = \frac{1}{\hbar} \bar{\nabla}_k E \Rightarrow \bar{\nabla}_k \bar{v} = \frac{1}{\hbar} \bar{\nabla}_k^2 E \\ \text{again } E = \frac{\hbar^2 k^2}{2m} &\Rightarrow \bar{\nabla}_k^2 E = \frac{\hbar^2}{m} \\ \therefore \bar{\nabla}_k \bar{v} &= \frac{\hbar}{m} \end{aligned} \right\}$$

$$-\frac{\bar{F}_{ext}}{m} \int f d^3k$$

recall $\int f d^3k = n$

$$-\frac{\bar{F}_{ext}}{m} n$$

Standard Drift-Diffusion Equation for Electrons/Holes-Text Version

$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\bar{\nabla}_x E \cdot \bar{\nabla}_k) \bar{v} d^3k + \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k - \int (f\bar{v} \cdot \bar{\nabla}_x) \bar{v} d^3k = -n \frac{\bar{v}}{\tau}$$

Assuming the mass is isotropic and constant and therefore:

$$f\bar{v}\bar{v} = f \begin{bmatrix} v_x^2 & 0 & 0 \\ 0 & v_y^2 & 0 \\ 0 & 0 & v_z^2 \end{bmatrix} = \frac{2}{m} \begin{bmatrix} fE_x & 0 & 0 \\ 0 & fE_y & 0 \\ 0 & 0 & fE_z \end{bmatrix} \quad \text{taking } E_x = E_y = E_z = E_i = \frac{1}{2}mv_i^2$$

$$\text{now } \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) = \frac{2}{m} \left[\frac{\partial fE_x}{\partial x} + \frac{\partial fE_y}{\partial y} + \frac{\partial fE_z}{\partial z} \right] = \frac{2}{m} [f\bar{\nabla}_x E_i + E_i \bar{\nabla}_x f]$$

$$\therefore \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k = \frac{2}{m} [n\bar{\nabla}_x E_i + E_i \bar{\nabla}_x n]$$

Assuming the material is isotropic i.e. temperature or energy is spatially independent

$$\therefore \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k = \frac{2}{m} [n\bar{\nabla}_x E_i + E_i \bar{\nabla}_x n] \xrightarrow{E_i = \frac{1}{3}\bar{E}} \frac{2}{3m} \bar{E} \bar{\nabla}_x n$$

Standard Drift-Diffusion Equation for Electrons/Holes-Text Version

$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\bar{\nabla}_x E \cdot \bar{\nabla}_k) \bar{v} d^3k + \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k - \int (f\bar{v} \cdot \bar{\nabla}_x) \bar{v} d^3k = -n \frac{\bar{v}}{\tau}$$

$$\frac{\partial(n\bar{v})}{\partial t} - \frac{\bar{F}_{ext}}{m} n + \frac{2}{3m} \bar{E} \bar{\nabla}_x n = -n \frac{\bar{v}}{\tau}$$

Notice that this term is completely ignored in the text

$\bar{F}_{ext} = -q\bar{F}$ where q = electronic charge, \bar{F} = field

$\bar{E} = \frac{3}{2} k_B T$, where T = temperature

$$\tau \frac{\partial(-qn\bar{v})}{\partial t} + (-qn\bar{v}) = \frac{q^2 \tau \bar{F}}{m} n + \frac{q\tau}{m} k_B T \bar{\nabla}_x n$$

electron current density = $J_n = -qn\bar{v}$
 electron mobility = $\mu_n = \frac{q\tau}{m}$

$$\tau \frac{\partial J_n}{\partial t} + J_n = nq\mu_n \bar{F} + \mu_n k_B T \bar{\nabla}_x n$$

Standard Drift-Diffusion Equation for Electrons/Holes-My Version

$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\bar{\nabla}_x E \cdot \bar{\nabla}_k) \bar{v} d^3k + \int \bar{\nabla}_x \cdot (f\bar{v}\bar{v}) d^3k - \int (f\bar{v} \cdot \bar{\nabla}_x) \bar{v} d^3k = -n \frac{\bar{v}}{\tau}$$

Identity: $\bar{G}\bar{\nabla} \cdot (g\bar{F}) = \bar{\nabla} \cdot (g\bar{F}\bar{G}) - (g\bar{F} \cdot \bar{\nabla})\bar{G}$

$$\int \bar{v} \bar{\nabla}_x \cdot (f\bar{v}) d^3k$$

Identity: $\bar{\nabla} \cdot (g\bar{F}) = \bar{F} \cdot \bar{\nabla}g + g\bar{\nabla} \cdot \bar{F}$

$$\int \bar{v} [f\bar{\nabla}_x \cdot \bar{v}] d^3k + \int \bar{v} [\bar{v} \cdot \bar{\nabla}_x f] d^3k$$

Recall $\bar{\nabla}_x \cdot \bar{v} = \frac{1}{\hbar} \bar{\nabla}_x \cdot \bar{\nabla}_k E = \frac{1}{\hbar} \bar{\nabla}_k \cdot \bar{\nabla}_x E$

$$\int \bar{v} \left[f \frac{1}{\hbar} \bar{\nabla}_k \cdot \bar{\nabla}_x E \right] d^3k + \int \bar{v} [\bar{v} \cdot \bar{\nabla}_x f] d^3k$$

Next Slide

Assuming the material is isotropic
i.e. energy is spatially independent $\bar{\nabla}_x E = 0$

Standard Drift-Diffusion Equation for Electrons/Holes-My Version

Previous Slide

$$\int \bar{v}\bar{v} \cdot \bar{\nabla}_x f d^3k$$

Assuming the mass is isotropic and constant and therefore:

$$\bar{v}\bar{v} = \begin{bmatrix} v_x^2 & 0 & 0 \\ 0 & v_y^2 & 0 \\ 0 & 0 & v_z^2 \end{bmatrix} = \frac{2}{m} \begin{bmatrix} E_x & 0 & 0 \\ 0 & E_y & 0 \\ 0 & 0 & E_z \end{bmatrix} \quad \text{taking } E_x = E_y = E_z = E_i = \frac{1}{2}mv_i^2$$

$$\text{now } \bar{v}\bar{v} \cdot \bar{\nabla}_x f = \frac{2E_i}{m} \left[\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} + \frac{\partial f}{\partial z} \right] = \frac{2}{m} [E_i \bar{\nabla}_x f]$$

$$\therefore \int \bar{v}\bar{v} \cdot \bar{\nabla}_x f d^3k = \frac{2}{m} [E_i \bar{\nabla}_x n]$$

$$\therefore \int \bar{v}\bar{v} \cdot \bar{\nabla}_x f d^3k = \frac{2}{m} [E_i \bar{\nabla}_x n] \xrightarrow{E_i = \frac{1}{3}\bar{E}} \frac{2}{3m} \bar{E} \bar{\nabla}_x n$$

Standard Drift-Diffusion Equation for Electrons/Holes-My Version

$$\frac{\partial(n\bar{v})}{\partial t} + \frac{1}{\hbar} \int (f\vec{\nabla}_x E \cdot \vec{\nabla}_k) \vec{v} d^3k + \int \vec{\nabla}_x \cdot (f\vec{v}\vec{v}) d^3k - \int (f\vec{v} \cdot \vec{\nabla}_x) \vec{v} d^3k = -n \frac{\bar{v}}{\tau}$$

$$\frac{\partial(n\bar{v})}{\partial t} - \frac{\vec{F}_{ext}}{m} n + \frac{2}{3m} \bar{E} \vec{\nabla}_x n = -n \frac{\bar{v}}{\tau}$$

As before in the text version

$$\tau \frac{\partial J_n}{\partial t} + J_n = nq\mu_n \vec{F} + \mu_n k_B T \vec{\nabla}_x n$$

ALTHOUGH BOTH THE TEXT VERSION AND MY VERSION ENDS UP WITH THE SAME ANSWER MY APPROACH IS ACCURATE SINCE IT ACCOUNTS FOR ALL THE TERMS IN THE GENERAL DRIFT-DIFFUSION EQUATION.

Drift-Diffusion Equation for Electron and Holes – And Finally

$$\text{Taking } \tau \frac{\partial J_n}{\partial t} + J_n = nq\mu_n \vec{F} + \mu_n k_B T \vec{\nabla}_x n$$

If the above equation is restricted to only zero order in J_n , then $\frac{\partial J_n}{\partial t} \sim 0$

$$\therefore J_n = nq\mu_n \vec{F} + \mu_n k_B T \vec{\nabla}_x n$$

Diffusion coeff (Einstein Relation) $D_n = \mu_n \frac{k_B T}{q}$



$$\therefore J_n = nq\mu_n \vec{F} + qD_n \vec{\nabla}_x n \dots \dots \dots (1)$$

Similarly, for holes (moves in opposite direction);

$$\therefore J_p = np\mu_p \vec{F} - pD_p \vec{\nabla}_x p \dots \dots \dots (2)$$

Equation (1) and (2) are the Drift-Diffusion Equations for Electrons and Holes respectively

Resources

- **Books**

- The Physics of Semiconductors, Kevin F. Brennan, Cambridge University Press, *New York* (1999)
- Introduction to Modern Statistical Mechanics, David Chandler, Oxford University Press, *New York* (1987)
- Introduction to Statistical Thermodynamics, Terrell L. Hill, Dover Publications Inc., *New York* (1986)

- **Websites**

- A great site hosted by the UIUC, Some great 1-D derivations in statistical mechanics
 - http://www-ncce.ceb.uiuc.edu/tutorials/bte_dd/html/bte_dd.html
- A good site with introductory derivations on statistical mechanics and some classical physics derivations, hosted by James Graham in UC-Berkeley
 - <http://astron.berkeley.edu/~jrg/ay202/lectures.html>
- The Mathworld® site. I find it one of the most helpful to check out theorems and formulae (I checked out the divergence theorem for this derivation)
 - <http://mathworld.wolfram.com/>

End of Lecture