Kinetic Transport Theory#3

Motion in a Concentration Gradient

The last driving "force" we consider with kinetic theory is a concentration gradient of charge carriers as represented in the open-circuited one-dimensional transported in the parallelapiped of Fig. 1. We assume $n_2 > n_1$ and expect that $J_n^{\,L} > J_n^{\,R}$ in this case since the perfectly randomizing nature of the collisions will cause more particles scatter from right-to-left than from left-to-right. Around the region bisected by z_0, we can define the difference between left and right-going carriers as,

$$J_n^{\,L} - J_n^{\,R} = \Delta J_{n,z} = -\frac{dJ_{n,z}}{dn}\frac{dn}{dz}\Delta z$$

where ΔJ_n is the net particle flux, also called the *diffusion current*. From the kinetic definition, $J_Z \equiv nv_z$, so that

$$\frac{dJ_{n,z}}{dn} = \upsilon_z$$

And we again apply a length scale equal to the mean-free-path, $\Delta x = \upsilon_x \tau$, so that

$$\Delta J_{n,z} = -\upsilon_z^{\,2}\tau\frac{dn}{dz}$$

If we take a spatial average (denoted by overbar) for the isotropic kinetic distribution,

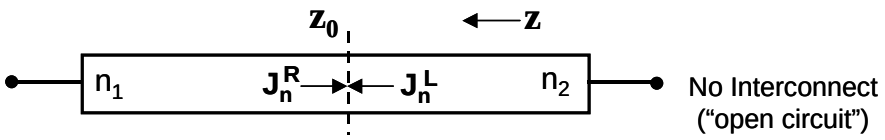

Fig. 1.

$$\overline{\Delta J_{n,z}} = -\overline{\upsilon_z^2}\,\tau\frac{dn}{dz} = -(1/3)v_0^2\tau\frac{dn}{dz} \equiv -D\frac{dn}{dz} \tag{1}$$

where the last step is motivated by the linear (response) relationship between ΔJ and dz, which leads us to call the proportionality constant the diffusivity,

$$D \rightarrow \text{diffusivity}\ \ D = \frac{1}{3}\upsilon_0^2\tau$$

Applying the Maxwell-Boltzman distribution and equipartition principle once again,

$$\frac{1}{2}m\upsilon_0^2 = \frac{3}{2}k_BT \ \text{ or } \ \upsilon_0^2 = \frac{3k_BT}{m}$$

So,
$$D = \frac{k_BT\tau}{m} = \frac{k_BT\mu}{e} \tag{2}$$

This is called the Einstein relation, and has a very special place in solid state materials, particularly semiconductor devices.[1] It is worth examining further by way of example. Let's take n-type silicon having a free electron concentration of n = $1x10^{16}$ cm^{-3} @ 300 K. Inspection of semiconductor tables shows that for this carrier concentration the conductivity of Si is σ ≈ 2.0/Ω-cm, which implies that μ ≈ 1250 cm^2/V-s and D ≈ 32 cm^2/s.

Potential Energy in Kinetic Theory

As in thermoelectric effect under open-circuit conditions, the gradient in *n* is usually associated with a built in electric field if the particles are charged. This motivates us to balance the diffusion current of (1) against a drift current, leading to

$$J_d = n\mu E \equiv -(-D\,dn/dx) \tag{3}$$

[1] Interestingly, Einstein's entry into science was largely through statistical mechanics and kinetic theory. And like his later endeavors in relativity, quantum theory, and unified field theory, he had a great knack for deriving incredibly elegant expressions based on the firm belief that physical laws should always be simple.

But from electrostatics, we also have $E = -\frac{d\phi}{dx}$ where ϕ is the electrostatic potential.

Combining this with Einstein's relation, (3) becomes

$$n\mu E = -n\mu \frac{d\phi}{dx} = \frac{k_B T \mu}{e} \frac{dn}{dx} \tag{4}$$

or,

$$-\frac{d\phi}{dx} = \frac{k_B T}{e} \frac{1}{n} \frac{dn}{dx}$$

This is a linear first-order differential equation in a single independent variable, so can be integrated immediately to get

$$\phi = -\frac{-k_B T}{e} \ln n + C$$

By taking the exponential of both sides, we get

$$n = \exp\left(-e\phi / k_B T\right) \exp(-eC / k_B T)$$

Because C is a constant of the integration, this can be re-written as

$$n = n_0 \exp\left(-e\phi / kT\right)$$

At first this might appear to be a trivial result since the kinetic theory provided the answer so easily. But it is a profound relationship for device physics since it suggests that the when diffusion and drift are occurring simultaneously in the open-circuit condition, the electrostatic potential has an exponential effect on the carrier concentration.

Multiple Scattering Events

Suppose that there are multiple scattering processes that are physically and statistically independent. We can write *Newton's equation* per particle as,

$$m\frac{d\upsilon}{dt}+m\left(\frac{\upsilon}{\tau_1}+\frac{\upsilon}{\tau_2}+\frac{\upsilon}{\tau_3}+\cdots+\frac{\upsilon}{\tau_n}\right)=qE$$

This is still a linear 1st order linear inhomogeneous differential equation with constant coefficients. So given an initial condition, say $\upsilon(t = 0) = \upsilon_0$, it can be solved uniquely. Generally the greatest number of scattering processes that one addresses is two. In this case,

$$\tau' \equiv \left(\frac{1}{\tau_1}+\frac{1}{\tau_2}\right)^{-1} \quad \text{or} \quad \tau' = \frac{\tau_1\tau_2}{\tau_1+\tau_2}$$

Newton's equation becomes

$$m\frac{d\upsilon}{dt}+m\frac{\upsilon}{\tau'}=qE$$

$$\upsilon=\upsilon_0 e^{-t/\tau'}+\frac{q}{e}\frac{e\tau' E}{m}(1-e^{-t/\tau'})$$

In the steady state $\upsilon \to \frac{q\tau' E}{m} \equiv \mu' E$, where $\mu' = \frac{e\tau'}{m}$. Furthermore, we can write the electrical current as $J_q = \sigma' E$, where $\sigma' = \frac{ne^2\tau'}{m}$, and

$$\rho' \equiv \frac{1}{\sigma'} = \frac{m}{ne^2\tau'} = \frac{m}{ne^2}\left(\frac{1}{\tau_1}+\frac{1}{\tau_2}\right) = \rho_1+\rho_2 \qquad (5)$$

The decomposition of total resistivity into independent components of (5) is called *Matthiessen's Rule*. In general, we can infer

$$\rho' = \sum_{i=1}^{N}\rho_i = \sum_{i=1}^{N}\frac{m}{ne^2\tau_i}$$

Refinements from Classical Scattering Theory

As we have derived it, kinetic theory is very useful at describing transport phenomena in

solids, but makes the following questionable assumptions:

(1) All particles in the population have the same scattering time τ that is independent of velocity and energy.

(2) Each particle in the population is statistically independent of the others in terms of velocity (energy) and position.

In reality, τ is dependent upon velocity (and energy) and the particles are statistically distributed and correlated through their quantum identity and the associated *Fermi statistics, Bose statistics or photon statistics*. In this case, the Newton's equations for two separate particles are not so simple, even if the particles are distinguishable. Intuitively, we should write the equations as

$$m\frac{d\upsilon_1(\upsilon_2)}{dt}+\frac{m\upsilon_1(\upsilon_2)}{\tau(\upsilon_1)}=F_1 \qquad\qquad m\frac{d\upsilon_2(\upsilon_1)}{dt}+\frac{m\upsilon_2(\upsilon_1)}{\tau(\upsilon_2)}=F_2$$

where $v_1(v_2)$ denotes the velocity of particle 1 as function of *v_2, and $v_2(v_1)$* denotes the velocity of particle 2 as function of *v_1.*

To estimate the velocity dependence of τ we start with collision theory (classical or quantum mechanical) for particles scattering in a force field (potential energy introduced). An important quantity is the collision or scattering rate, f_S

$$f_S = n\sigma_S(\upsilon)\cdot\upsilon \equiv \frac{1}{\tau}$$

where N_S is the density of scattering centers, $\sigma_S(v)$ is the their scattering cross section, and v is the velocity of the particles. For example, consider ionized impurity scattering (which is common in doped semiconductors, even at room temperature). Early work in particle physics by Rutherford and others showed that high-energy particles experience much less scattering

from charged centers than low energy ones. They found,

$$\sigma_S(\upsilon) = \frac{A}{\left(U_K^*\right)^2} \equiv \frac{A}{\left[(1/2)m\upsilon^2\right]^2}$$

where A is a constant dependent on the force field and the particle in question.

So, $$\tau_s = \frac{1}{N_S \sigma_S \upsilon} = \frac{\left((1/2)m\upsilon^2\right)^2}{AN_S\upsilon} = \frac{(m/2)^2\upsilon^3}{AN_S}$$

This is a very strong velocity dependence. If we assume for the moment that the scattered particles are Maxwell-Boltzmann distributed so the equipartition law applies, then,

$\upsilon^3 = (3k_BT/m)^{3/2}$, and

$$\tau_S = \frac{(m/2)^2 \left(3k_B/m\right)^{3/2} T^{3/2}}{AN_S}$$

This characteristics "$T^{3/2}$" law shows up surprisingly often in the mobility of semiconductors and certain dielectric materials. And it is usually a sign of ionized impurity or defect scattering.