In last lecture, we talked about the Newton's shear stress law.

U
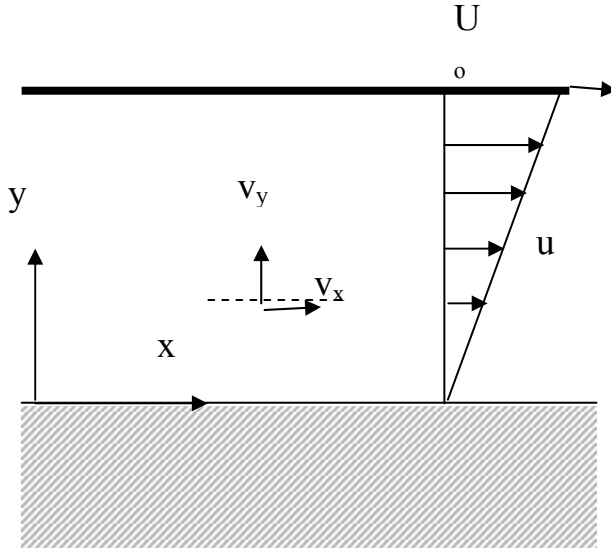
Assuming that the number density of particles is n, the number density of particles having velocity **v** is

$$f_o(v_x, v_y, v_z) = nP(v_z, v_y, v_z) = n\left(\frac{m}{2\pi\kappa_B T}\right)^{3/2} e^{-m\left[(v_x - u)^2 + v_y^2 + v_z^2\right]/2\kappa_B T}$$

From $f = f_o - \tau\left(\mathbf{v} \bullet \nabla_{\mathbf{r}} f_o + \frac{\mathbf{F}}{m} \bullet \nabla_{\mathbf{v}} f_o\right)$ (**F** is zero here because this is no external fields here and gravity is neglected), the distribution function is

$$f = f_o - \tau\left(v_x \hat{i} + v_y \hat{j} + v_z \hat{k}\right) \cdot \left(\frac{\partial f_o}{\partial x}\hat{i} + \frac{\partial f_o}{\partial y}\hat{j} + \frac{\partial f_o}{\partial z}\hat{k}\right) = f_o - \tau v_y \frac{\partial f_o}{\partial y} = f_o - \tau v_y \frac{\partial f_o}{\partial u}\frac{\partial u}{\partial y}.$$

Note: We can also prove $u = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v_x f dv_x dv_y dv_z$.

The shear stress along the x-direction, on a plane perpendicular y-axis can be calculated by considering the momentum exchange across the plane,

$$\tau_{xy} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v_y [mv_x] f dv_x dv_y dv_z$$

$$= -\frac{\partial u}{\partial y}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\tau v_y^2 mv_x \frac{\partial f_o}{\partial u} dv_x dv_y dv_z = \mu\frac{\partial u}{\partial y}$$

The dynamic viscosity can be

$$\mu = -\int\int\int \tau v_y^2 (mv_x)\frac{\partial f_o}{\partial u} dv_x dv_y dv_z$$

$$= m^2 \tau n \left(\frac{m}{2\pi\kappa_B T} \right)^{3/2} \int_{-\infty}^{\infty} e^{-mv_z^2/(2\kappa_B T)} dv_z \int_{-\infty}^{\infty} v_y^2 e^{-mv_y^2/(2\kappa_B T)} dv_y \int_{-\infty}^{\infty} \frac{v_x'^2}{\kappa_B T} e^{-mv_x'^2/(2\kappa_B T)} dv_x' \ .$$
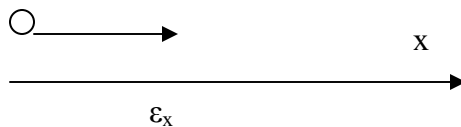
Note: Two integrations are used to calculate the above equation:

(1) $\left(\int_{-\infty}^{+\infty} e^{-x^2} dx \right)^2 = \left(\int_{-\infty}^{+\infty} e^{-x^2} dx \right)\left(\int_{-\infty}^{+\infty} e^{-y^2} dy \right) = \int_{-\infty}^{+\infty} e^{-(x^2+y^2)} dxdy = \int_0^{+\infty} e^{-r^2} 2\pi r dr$ yields

$\int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi}$.

(2) $f(a) = \int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\dfrac{\pi}{a}}$ leads to $f'(a) = -\int_{-\infty}^{+\infty} x^2 e^{-ax^2} dx = \left(\sqrt{\dfrac{\pi}{a}} \right)' = -\dfrac{\sqrt{\pi}}{2} a^{-3/2}$.
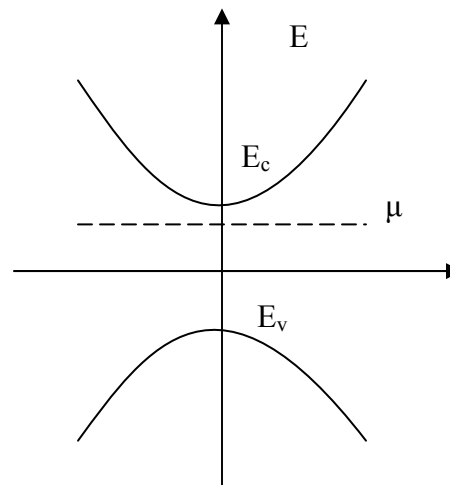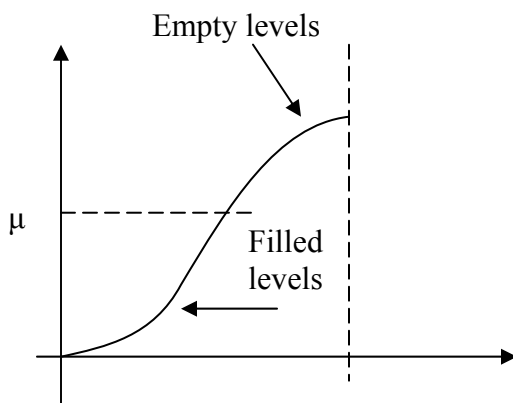
Ohm's Law

x

ε_x

Now f_o obeys the Fermi-Dirac distribution

$$f_o(E, E_f, T) = \frac{1}{\exp\left(\dfrac{E - \mu}{\kappa_B T} \right) + 1} \ ,$$

and $f = f_o - \tau \left(\mathbf{v} \bullet \nabla_{\mathbf{r}} f_o + \dfrac{\mathbf{F}}{m} \bullet \nabla_{\mathbf{v}} f_o \right)$ becomes

$$f = f_o - \tau \left(v_x \frac{df_o}{dx} + \frac{q\varepsilon_x}{m} \frac{\partial f_o}{\partial E} \frac{\partial E}{\partial v_x} \right).$$

Empty levels

Filled levels

μ

E

E_c

μ

E_v

For metals (left figure), the electrons fill part of the band, while the Fermi level normally lies within the band gap for semiconductors. In the latter situation, the parabolic approximation is used

$$E = E_c + \frac{1}{2}\frac{\hbar^2 k^2}{m^*} = E_c + \frac{1}{2}m^*\left(v_x^2 + v_y^2 + v_z^2\right),$$

thus

$$f = f_o - \tau\left(v_x \frac{\partial f_o}{\partial x} + \frac{q\varepsilon_x}{m}\frac{\partial f_o}{\partial E}\frac{\partial E}{\partial v_x}\right) = f_o - \tau v_x\left(\frac{\partial f_o}{\partial x} + q\varepsilon_x \frac{\partial f_o}{\partial E}\right).$$

The current density (A/m²) is then

$$J_q = \frac{1}{V}\sum_{k_z=-\infty}^{\infty}\sum_{k_y=-\infty}^{\infty}\sum_{k_z=-\infty}^{\infty} qv_x f = \frac{1}{(2\pi)^3}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} qv_x f dk_x dk_y dk_z$$

Changing to spherical coordinate system ($dk_x dk_y dk_z = k^2 \sin\theta d\theta d\varphi dk$) and rewrite the above equation with $D(E)$ yields

$$J_q = \int_0^{2\pi}\int_0^{\pi}\int_0^{+\infty} qv_x f \frac{D(E)}{4\pi}\sin\theta d\theta d\varphi dE$$

$$= -\frac{q}{3}\int_0^{\infty} \tau v^2 D(E)\left(\frac{\partial f_o}{\partial x} + q\varepsilon_x \frac{\partial f_o}{\partial E}\right)dE \quad .$$

Now we let E$_c$=0 be the reference energy level. And the distribution becomes

$$f_o\left(E, E_f, T\right) = \frac{1}{\exp\left(\dfrac{E_k - (\mu - E_c)}{\kappa_B T}\right) + 1},$$

where E$_k$ denotes the kinetic energy.

Noticing $\dfrac{\partial f_0}{\partial T} = -\dfrac{E_k - \mu}{T}\dfrac{\partial f_0}{\partial E_k}$, $\dfrac{\partial f_0}{\partial \mu} = -\dfrac{\partial f_0}{\partial E_k}$, we have

$$\frac{\partial f_0}{\partial x} = \frac{\partial f_0}{\partial \mu}\frac{\partial \mu}{\partial x} + \frac{\partial f_0}{\partial T}\frac{\partial T}{\partial x}$$

$$= -\frac{\partial f_0}{\partial E_k}\frac{\partial \mu}{\partial x} - \frac{E_k - \mu}{T}\frac{\partial f_0}{\partial E_k}\frac{\partial T}{\partial x}$$

Note: Defining $y = \dfrac{E_k - \mu}{\kappa_B T}$, $f_o\left(E, E_f, T\right) = \dfrac{1}{\exp(y) + 1}$, we can observe

$$\frac{\partial f_0}{\partial T} = -\frac{E_k - \mu}{T}\frac{\partial f_0}{\partial E_k}$$

from

$$\frac{\partial f_0}{\partial T} = -\frac{\partial f_0}{\partial y}\frac{E_k - \mu}{k_B T^2}, \quad \frac{\partial f_0}{\partial E_k} = \frac{\partial f_0}{\partial y}\frac{1}{k_B T}.$$

The flux is thus

$$J_q = -\frac{q}{3}\int_0^\infty \tau v^2 \left(-\frac{\partial \mu}{\partial x} - \frac{E_k - \mu}{T}\frac{\partial T}{\partial x} + q\varepsilon_x \right)\frac{\partial f_0}{\partial E_k}D(E_k)dE_k$$

$$= \left\{ \frac{1}{3}\int_0^\infty q\tau v^2 \frac{\partial f_0}{\partial E_k}D(E_k)dE_k \right\}\left(\frac{\partial \mu}{\partial x} - q\varepsilon_x \right) + \left\{ \frac{1}{3}\int_0^\infty q\tau v^2 \left(\frac{E_k - \mu}{T} \right)\frac{\partial f_0}{\partial E_k}D(E_k)dE_k \right\}\frac{\partial T}{\partial x}$$

Discussion

To simplify, let $L_{11} = \frac{1}{3}\int_0^\infty q\tau v^2 \frac{\partial f_0}{\partial E_k}D(E_k)dE_k$.

1) $\partial T/\partial x = 0$ (isothermal), we have

$$J_x = L_{11}\left(\frac{\partial \mu}{\partial x} - q\varepsilon_x \right) = L_{11}q\frac{\partial \phi}{\partial x} ,$$
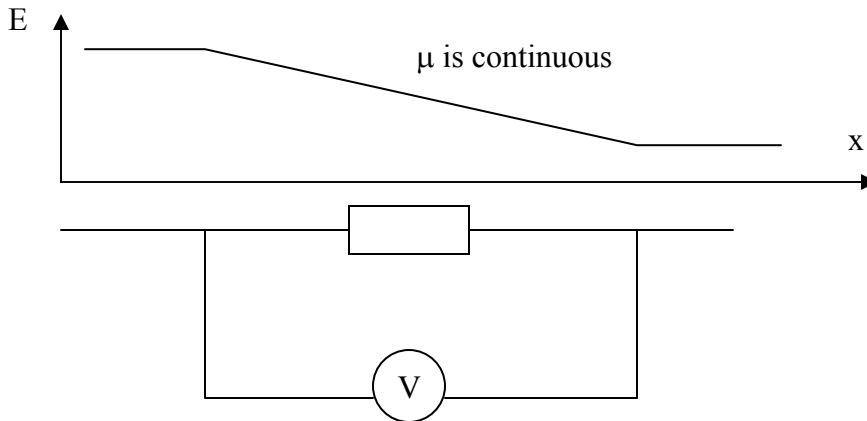
where $\phi = \frac{\mu}{q} + v$ is the electrochemical potential.

Note: $\frac{\partial \mu}{\partial x} - q\varepsilon_x = \frac{\partial \mu}{\partial x} + q\frac{dV}{dx} = \frac{\partial}{\partial x}\left(\frac{\mu}{q} + v \right).$

The flux is often written as

$$J_x = qn\mu_e\varepsilon_x + Dq\frac{\partial n}{\partial x}$$

where the first term corresponds to drift, the second term denotes diffusion; μ_e is called the **mobility** [$m^2V^{-1}s^{-1}$] and D is the **diffusivity** [m^2s^{-1}], n is carrier concentration. In the following figures, we actually measure both terms in the above equation.

Note: Recall we use $n = \int fD(E)dE$ to determine μ in Lecture 11. Normally n is related to μ. In semiconductors, when we increase doping, n will increase while μ will drop due to scattering. In metals, the large n is almost constant and $J_e = qn\mu_e\varepsilon_x = \sigma\varepsilon_x$.

In non-degenerate semiconductors, the Fermi-Dirac distribution can be approximated by the Boltzmann distribution and $D = k_B T \mu / q$, called Einstein relationship. This name comes because it is derived following Einstein's work on Brownian motions.

2) $\partial T / \partial x \neq 0$
Now the equation is written as
$$J_x = L_{11} q \left(\frac{d\Phi}{dx} \right) + L_{21} \left(\frac{dT}{dx} \right).$$
For open circuits (zero flux), we have
$$0 = L_{11} q \left(\frac{d\Phi}{dx} \right) + L_{21} \left(\frac{dT}{dx} \right),$$
thus
$$\frac{d\Phi}{dx} = -\frac{L_{12}}{L_{11}} \frac{dT}{dx} = -S \frac{dT}{dx},$$
where $S = \dfrac{L_{12}}{L_{11}}$ (VK^{-1}) is called **Seebeck coefficient**. The Seebeck voltage is the steady-state voltage accumulated under the open circuit condition. If the conductor is a uniform material such that S is a constant, the voltage difference does not dependent on the temperature profile. This is the principle behind the thermocouple for temperature measurements. A thermocouple (the following figure) employs two conductors for the easy of measuring the voltage difference.
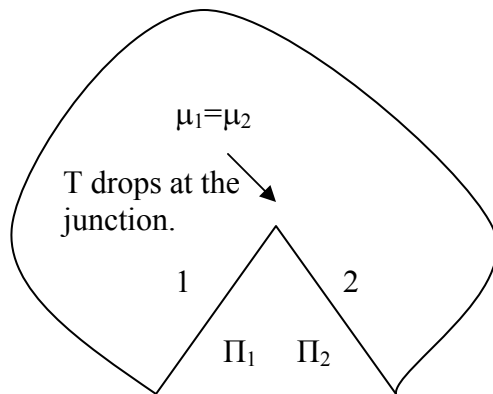
For the heat flux, we have
$$dE = dq + \mu dn,$$
$$J_q = \sum \sum \sum 2(E - \mu) v_x f = L_{21} \frac{d\phi}{dx} + L_{22} \frac{dT}{dx}.$$

The heat flux is also written as $J_q = \Pi J_x$, in which the Peltier factor $\Pi = ST$.