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Lecture XXX

Approximation Solutions to Boltzmann Equation: Relaxation Time Approximation

Readings: Brennan Chapter 6.2 & Notes

Approximation Solutions of the Boltzmann Equation (Section 6.2)

General Solution

General Boltzmann equation (BTE) is

$$\boxed{\frac{\partial f}{\partial t}+\frac{\vec{F}_{ext}}{\hbar}\cdot\vec{\nabla}_k f+\vec{v}\cdot\vec{\nabla}_x f=-\int \begin{matrix}\{f(x,k,t)[1-f(x,k',t)]S(k,k') \\ -f(x,k',t)[1-f(x,k,t)S(l',k)\}\end{matrix} dk'} \qquad (1)$$

which is a integral-differential equation. In order to find the solution, drastic approximations have to be used, which are often invalid for the particular situation. Therefore, a technique based on the relaxation time approximation is use to solve for the Boltzmann equation. It should be noted that this approximation does not always work, but because it greatly reduces the complexity of the Boltzmann equation and a closed form solution can be obtained, it will be investigated here. For cases that the approximation can not be used, more sophisticated methods such as drift-diffusion and the Monte Carlo method (Section 6.3) should be used.

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Issues (how to solve it?)

The problem with the Boltzmann equation is the integral scattering term. As a approximation, let's replace it with a constant relaxation term, which reduces the original integral-differential equation into only a differential equation. In addition, the partial derivative of the distribution function with respect to time due to collisions is assumed to be inversely proportional to a lifetime that characterizes the mean free time between collisions. Hence, if f_o is the equilibrium distribution function and f is the nonequilibrium distribution function for which the Boltzmann equation is solved, the left hand side of the Boltzmann equation changes to

$$\boxed{\left(\frac{\partial f}{\partial t}\right)_{collisions} = -\frac{f - f_o}{\tau}} \qquad (2)$$

Equation (2) shows that the system will relax to equilibrium after time τ, which is the relaxation time and represents the average time it takes for the system to relax from the nonequilibrium state to the equilibrium state through collisions.

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Further Investigation

Apply electric field F_o with $\nabla_x f = 0$ (no diffusion gradient), at t<0 Boltzmann equation becomes

$$\frac{\partial f}{\partial t} = -\frac{q\vec{F}_o}{m} \cdot \vec{\nabla}_v f(x,v,t) + \left(\frac{\partial f}{\partial t}\right)_{collisions} \quad (3)$$

then F_o is removed, so for t>0 Boltzmann equation reduces to

$$\left(\frac{\partial f}{\partial t}\right) = \left(\frac{\partial f}{\partial t}\right)_{collisions} \quad (4)$$

Using (2) and adding f_o into the derivative (since $\frac{\partial f_o}{\partial t} = 0$),

$$\frac{\partial}{\partial t}(f - f_o) = -\frac{f - f_o}{\tau} \quad (5)$$

the above differential equation is solved through

$$y \equiv (f - f_o) \qquad \frac{dy}{dt} = -\frac{y}{t} \qquad y = y_o e^{\frac{t}{\tau}} \quad (6)$$

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Further Investigation (Cont'd)

After substituting (6) into (5), (5) evaluates to

$$\boxed{f(t) = f_o + [f(0) - f_o]e^{-\frac{t}{\tau}}} \qquad (7)$$

From the above results, it's clear that as t→∞, f relaxes to f_o, however, the system doesn't need that much time, it will achieve equilibrium when t=τ.

Again, how does the system relax? (Clemson student's answer: by sitting on the couch?)

The system completely relaxes through scattering(collision) events. If scattering doesn't take place, the rate change(8) of the nonequilibrium state becomes zero, which means that there is no possible solution for (7) such that f will relax to f_o .

$$\frac{\partial f}{\partial t} = 0 \qquad (8)$$

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Uniform Electric Field

Uniform electric field is applied to a steady state system such that there's no spatial gradient, hence

$$\nabla_x f = 0 \qquad \frac{\partial f}{\partial t} = 0 \tag{9}$$

before approximations the BTE is

$$\boxed{\frac{\partial f}{\partial t} + \frac{\vec{F}_{ext}}{\hbar} \cdot \vec{\nabla}_v f + \vec{v} \cdot \vec{\nabla}_x f = \left(\frac{\partial f}{\partial t}\right)_{collisions}} \tag{10}$$

with the above assumptions, the BTE becomes

$$\frac{\vec{F}_{ext}}{m} \cdot \vec{\nabla}_v f = \left(\frac{\partial f}{\partial t}\right)_{collisions} = -\frac{f - f_o}{\tau} \tag{11}$$

$$\boxed{\vec{F}_{ext} = -q\vec{F}_o}$$

$$\Rightarrow \qquad \frac{-q\vec{F}_o \cdot \vec{\nabla}_v f}{m} = -\frac{f - f_o}{\tau} \tag{12}$$

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Uniform Electric Field (Cont'd)

Assume field is only in z direction, and f is not far from f_o , which can be equated to the Maxwellian.

$$\frac{qF_o\tau}{m}\frac{\partial f}{\partial v_z} = f - f_o \qquad \frac{\partial f}{\partial v_z} \sim \frac{\partial f_o}{\partial v_z} \qquad f_o = e^{-\frac{mv^2}{2k_bT}} \tag{13}$$

$$\Rightarrow \frac{\partial f}{\partial v_z} = \frac{\partial f_o}{\partial v_z} = \frac{\partial}{\partial v_z} e^{-\frac{mv^2}{2k_BT}} = -\frac{mv_z}{k_BT} e^{-\frac{mv^2}{2k_BT}} \tag{14}$$

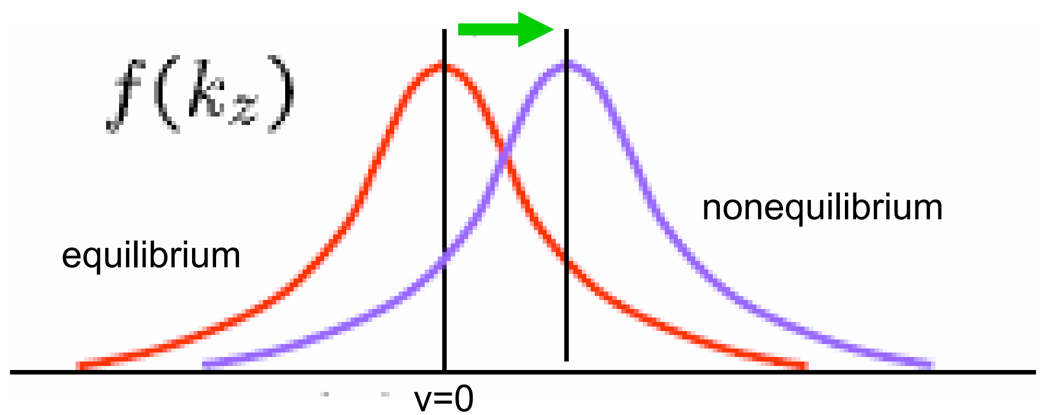
$$\Rightarrow -\frac{qF_o\tau}{m}\frac{mv_z}{k_BT} e^{-\frac{mv^2}{2k_BT}} = f - f_o \quad \Rightarrow \quad -\frac{qF_o\tau}{k_BT} v_z f_o = f - f_o \tag{15}$$

$$\Rightarrow \quad f = f_o\left[1 - \frac{qF_o v_z \tau}{k_BT}\right] \quad \Rightarrow \quad \boxed{f = f_o\left[1 - \frac{qF_o(v\cos\theta)\tau}{k_BT}\right]} \tag{16}$$

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Uniform Electric Field (Cont'd)

Equation (16) completely describes the distribution function of the nonequilibrium state, and it is clear that the nonequilibrium state is just shifted version of the equilibrium state (Figure 6.2.1 in book), whereas the equilibrium distribution function is centered about v=0 (avg. v=0).



So why is this "slight" shift so important?

The current density was determined for the equilibrium case earlier (current density is zero at equilibrium), but with the shift in the distribution the current density for the nonequilibrium case becomes non-zero.

Approximation Solutions of the Boltzmann Equation (Section 6.3)

Current Density

Current density is defined as

$$j_z = -nq\vec{v}_z \qquad (17)$$

the average velocity for the nonequilibrium case is not zero, so current density is not zero.

$$\bar{v}_z = \frac{\int v_z f(v) D(v) d^3v}{\int f(v) D(v) d^3v} \qquad D(v)d^3v = \frac{2m^3 Vol}{h^3} dv_x dv_y dv_z \qquad (18)$$

$$\Rightarrow \quad \bar{v}_z = \frac{\int_0^\infty \int_0^\pi \int_0^{2\pi} d\phi f_o(v) \left[1 - \frac{qF_o \tau v \cos\theta}{k_B T}\right] v \cos\theta v^2 dv \sin\theta d\theta}{\int_0^\infty \int_0^\pi \int_0^{2\pi} d\phi f_o(v) \left[1 - \frac{qF_o \tau v \cos\theta}{k_B T}\right] v^2 dv \sin\theta d\theta} \qquad (19)$$

$$\boxed{\int_0^\pi \cos\theta \sin\theta d\theta = 0}$$

$$\Rightarrow \quad \bar{v}_z = \frac{-\int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{f_o(v) qF_o \tau v^4 \cos^2\theta \sin\theta}{k_B T} d\theta dv}{\int_0^\infty \int_0^\pi \int_0^{2\pi} f_o(v) v^2 \sin\theta dv d\theta} \qquad (20)$$

Approximation Solutions of the Boltzmann Equation (Section 6.3)

Current Density (Cont'd)

$$\boxed{\int_0^{\pi} \cos^2\theta \sin\theta d\theta = 2/3}$$

$$\boxed{\int_0^{\pi} \sin\theta d\theta = 2}$$

$$\Rightarrow \quad \bar{v}_z = \frac{-\frac{1}{3}\frac{qF_o}{k_B T}\int_0^{\infty} v^2\tau(v)v^2 f_o(v)dv}{\int_0^{\infty} v^2 f_o(v)dv} \quad \Rightarrow \quad \bar{v}_z = -\frac{qF_o}{3k_B T}\overline{v^2\tau(v)} \qquad (21)$$

$$\boxed{\overline{\frac{1}{2}mv^2} = \frac{3}{2}k_B T \Rightarrow k_B T = \frac{1}{3}m\overline{v^2} \Rightarrow \frac{3k_B T}{mv^2} = 1}$$

$$\Rightarrow \quad \bar{v}_z = -\frac{qF_o}{3k_B T}\overline{v^2\tau(v)}\frac{3k_B T}{mv^2} \quad \Rightarrow \quad \bar{v}_z = -\frac{qF_o}{m}\frac{\overline{v^2\tau}}{\overline{v^2}} = -\frac{qF_o}{m}\bar{\tau} \qquad (22)$$

$$\Rightarrow \quad \boxed{j_z = -nq\bar{v}_z = \frac{nq^2 F_o\bar{\tau}}{m} = \sigma F_o} \qquad (23)$$

$$\boxed{\sigma = \frac{nq^2\bar{\tau}}{m} = nqu} \qquad (24)$$

Approximation Solutions of the Boltzmann Equation (Section 6.3)

Current Density (Cont'd)

$$\boxed{u = \left| \frac{\bar{v}_z}{F_o} \right| = \frac{q\bar{\tau}}{m}} \qquad (25)$$

From equation (23), the current density for a nonquilibrium state is not zero and the subsequent parameters of electron mobility u (25) and conductivity σ (24) are also derived for the nonequilibrium case.

Approximation Solutions of the Boltzmann Equation (Section 6.2)

Example

Consider a uniform isotropic substance at constant temperature in the presence of a constant applied electric field F. If steady state conditions are achieved, the nonequilibrium distribution function can be written as

$$f = f_o(1+\lambda)$$

Determine the parameter λ.

Solution: Remember that if an uniform electric field is applied un steady state conditions,

$$f = f_o\left[1 - \frac{qF_o(v\cos\theta)\tau}{k_B T}\right]$$

$$\Rightarrow \quad f_o(1+\lambda) = f_o\left[1 - \frac{qF_o(v\cos\theta)\tau}{k_B T}\right]$$

$$\Rightarrow \quad \lambda = -\frac{qF_o(v\cos\theta)\tau}{k_B T}$$

Can you find the current density???