Physics 740: Spring 2006: 02/05/07

P740.3.tex

A. The Boltzmann Equation. The Boltzmann equation in the relaxation time approximation to the collision term is

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = -\frac{f - f_0}{\tau}, \tag{1}$$

where $f = f(\mathbf{x}, \mathbf{p}, t)$ is the density of particles at $(\mathbf{x}, \mathbf{p})$ at time t and

1. $f_0 = f_0(\mathbf{x}, \mathbf{p})$ is the equilibrium distribution function at $(\mathbf{x}, \mathbf{p})$,
2. $\nabla_{\mathbf{x}} = \partial/\partial\mathbf{x}$ and $\nabla_{\mathbf{p}} = \partial/\partial\mathbf{p}$,
3. τ is the relaxation time, a characteristic time for departures from equilibrium to return to equilibrium.

This equation is space-time local, i.e., the equilibrium distribution function can vary from place to place, can vary *slowly* in time. The variations in space are on a scale large compared to the mean free path, the variations in time are slow compared to τ.

The proper venue for deriving the Boltzmann equation from a more fundamental description is non-equilibrium statistical physics, where one starts with the Liouville equation for the density in classical phase space. If you are interested **http://denali.phys.uniroma1.it/ puglisi/thesis/node20.html**.

B. Uses for $f(\mathbf{x}, \mathbf{p}, t)$.

1. Calculate local averages

$$< A(t) >= \frac{\int d\mathbf{x} \int d\mathbf{p}\ A(\mathbf{x}, \mathbf{p}) f(\mathbf{x}, \mathbf{p}, t)}{\int d\mathbf{x} \int d\mathbf{p}\ f(\mathbf{x}, \mathbf{p}, t)}. \tag{2}$$

2. Find an equation of motion for the average of A, e.g.,

$$\frac{\partial < A >}{\partial t} + \cdots, \tag{3}$$

see below.

C. Examples of $f_0(\mathbf{x}, \mathbf{p})$.

1. ideal gas of N particles, in a uniform space of volume V, in contact with a temperature reservoir at T:

$$f_0(\mathbf{x}, \mathbf{p}) = \frac{N}{V} I_0^{-3} exp\left(-\beta \frac{\mathbf{p}^2}{2m}\right), \tag{4}$$

$$n(\mathbf{x}) = \int d\mathbf{p}\ f_0(\mathbf{x}, \mathbf{p}) = \frac{N}{V}, \tag{5}$$

$$1 = \int d\mathbf{p}\ I_0^{-3} exp\left(-\beta \frac{\mathbf{p}^2}{2m}\right). \tag{6}$$

2. ideal gas of N particles, each particle confined by the single particle potential $U(\mathbf{x})$, in contact with a temperature reservoir at T:

$$f_0(\mathbf{x}, \mathbf{p}) = N I_U^{-1} I_0^{-3} exp\left(-\beta \left[\frac{\mathbf{p}^2}{2m} + U(\mathbf{x})\right]\right), \tag{7}$$

$$n(\mathbf{x}) = \int d\mathbf{p}\ f_0(\mathbf{x}, \mathbf{p}) = N I_U^{-1} exp\left(-\beta U(\mathbf{x})\right), \tag{8}$$

$$1 = \int d\mathbf{p}\ I_0^{-3} exp\left(-\beta \frac{\mathbf{p}^2}{2m}\right), \tag{9}$$

$$1 = \int d\mathbf{x}\ I_U^{-1} exp\left(-\beta U(\mathbf{x})\right). \tag{10}$$

3. ideal gas of N particles, with average x-momentum P, in a uniform space of volume V, in contact with a temperature reservoir at T:

   (a)

$$f_0(\mathbf{x}, \mathbf{p}) = \frac{N}{V} I_0^{-2} I_Q^{-1} exp\left(-\beta \left[\frac{\mathbf{p}^2}{2m} - Q p_x\right]\right), \tag{11}$$

$$n(\mathbf{x}) = \int d\mathbf{p}\ f_0(\mathbf{x}, \mathbf{p}) = \frac{N}{V}, \tag{12}$$

$$1 = \int d\mathbf{p}\ I_0^{-2} I_Q^{-1} exp\left(-\beta \left[\frac{\mathbf{p}^2}{2m} - Q p_x\right]\right). \tag{13}$$

   (b)

$$P = < p_x > = \frac{1}{\beta} \frac{d}{dQ} ln I_Q, \tag{14}$$

$$I_Q = \int dp\ exp\left(-\beta \left[\frac{p^2}{2m} - Q p\right]\right). \tag{15}$$

   (c) the symmetry $\mathbf{p} \rightarrow -\mathbf{p}$ is broken by the Q term, consequently $< p_x >$ is non-zero. How is Q related to $< p_x > = P$?

D. An equation of motion for $< A >$. Define

$$n = n(\mathbf{x}, t) \; = \; \int d\mathbf{p}\; f(\mathbf{x}, \mathbf{p}, t), \tag{16}$$

$$< A > = < A(\mathbf{x}, t) > \; = \; \frac{\int d\mathbf{p}\; A f(\mathbf{x}, \mathbf{p}, t)}{\int d\mathbf{p}\; f(\mathbf{x}, \mathbf{p}, t)}. \tag{17}$$

Note. In this section $< \cdots >$ is an average over $\mathbf{p}$ *only!!!*

For A independent of t multiply Eq. (1) by A and integrate on $\mathbf{p}$:

1. first term in Eq. (1)

$$\int d\mathbf{p}\; A\; \frac{\partial f}{\partial t} = \frac{\partial\; (n < A >)}{\partial t} = \frac{\partial < nA >}{\partial t}. \tag{18}$$

2. second term in Eq. (1)

$$\int d\mathbf{p}\; A\; (\mathbf{v} \cdot \nabla_{\mathbf{x}})\; f = \nabla_{\mathbf{x}} \cdot < nA\mathbf{v} > - < n\mathbf{v} \cdot \nabla_{\mathbf{x}} A >, \tag{19}$$

   [use $\nabla \cdot (A\mathbf{v}f) = f\; \mathbf{v} \cdot \nabla A + A\; \mathbf{v} \cdot \nabla f$].

3. third term in Eq. (1)

$$\int d\mathbf{p}\; A\; (\mathbf{F} \cdot \nabla_{\mathbf{p}})\; f \; = \; \int d\mathbf{p}\; \nabla_{\mathbf{p}} \cdot (A\mathbf{F}f) - \int d\mathbf{p}\; Af\nabla_{\mathbf{p}} \cdot \mathbf{F}) - < n\mathbf{F} \cdot \nabla_{\mathbf{p}} A >, \tag{20}$$

$$= \; - < n\mathbf{F} \cdot \nabla_{\mathbf{p}} A >, \tag{21}$$

   where the simplification occurs because the first integral goes to a surface in $\mathbf{p}$-space that can be arbitrarily far away (where $f = 0$) and we assume the applied forces are independent of $\mathbf{p}$ (re-think this if velocity dependent forces are involved).

4. assume that A is a quantity that is conserved by the collision process so that the term on the RHS of Eq. (1) is dropped.

Assemble the pieces

$$\frac{\partial < nA >}{\partial t} + \nabla_{\mathbf{x}} \cdot < nA\mathbf{v} > \; - \; < n\mathbf{v} \cdot \nabla_{\mathbf{x}} A > - < n\mathbf{F} \cdot \nabla_{\mathbf{p}} A > = 0, \tag{22}$$

$$\frac{\partial < nA >}{\partial t} + \nabla_{\mathbf{x}} \cdot < nA\mathbf{v} > \; - \; n < \mathbf{v} \cdot \nabla_{\mathbf{x}} A > - n\; \mathbf{F} \cdot < \nabla_{\mathbf{p}} A > = 0, \tag{23}$$

where the second line is a possibly convenient re-arrangement. The quantity $< nA >$ is a density and $< nA\mathbf{v} >$ the corresponding current.

E. **Conservation laws**. Make 5 choices for A, $A = m, mv_i$ $(i = x, y, z)$, kinetic energy.

1. $A = m$, $\rho = mn$, $\mathbf{J}_\rho =< \rho \mathbf{v} >= \rho < \mathbf{v} >= \rho \mathbf{u}$,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J}_\rho = 0. \tag{24}$$

2. $A = mv_i$,

$$\frac{\partial < \rho v_i >}{\partial t} + \sum_k \frac{\partial < \rho v_i v_k >}{\partial x_k} = \frac{1}{m} \rho F_i. \tag{25}$$

massage. Use $< \rho v_i >= \rho u_i$ and

$$v_i v_k \;=\; (v_i - u_i)(v_k - u_k) + v_i u_k + v_k u_i - u_i u_k, \tag{26}$$

$$< \rho v_i v_k >= \rho < v_i v_k > \;=\; \rho < (v_i - u_i)(v_k - u_k) > + \rho u_i u_k, \tag{27}$$

to write

$$\frac{(\partial \rho u_i)}{\partial t} + \sum_k \frac{\partial (\rho u_i u_k)}{\partial x_k} = \frac{1}{m} \rho F_i - \sum_k \frac{\partial}{\partial x_k} \rho < (v_i - u_i)(v_k - u_k) > . \tag{28}$$

Define the pressure tensor

$$P_{ik} = \rho < (v_i - u_i)(v_k - u_k) > \tag{29}$$

and find

$$\frac{\partial u_i}{\partial t} + \mathbf{u} \cdot \nabla u_i = \frac{1}{m} F_i - \sum_k \frac{1}{\rho} \frac{\partial P_{ik}}{\partial x_k}. \tag{30}$$

[To get here from Eq. (27) we used Eq. (23) to get rid of the derivatives of ρ.]

3. $A = m|\mathbf{v} - \mathbf{u}|^2/2$, this is the kinetic energy in the motion of the particles in the gas relative to the local average velocity, an energy that will be identified with the temperature.

$$\frac{1}{2} \frac{\partial}{\partial t} < \rho |\mathbf{v} - \mathbf{u}|^2 > + \frac{1}{2} \sum_k \frac{\partial}{\partial x_k} < \rho v_k |\mathbf{v} - \mathbf{u}|^2 > - \frac{1}{2} \rho \sum_k < v_k \frac{\partial}{\partial x_k} |\mathbf{v} - \mathbf{u}|^2 >= 0. \tag{31}$$

massage. Define (think $E = (3/2) k_B T$, $\theta \leftrightarrow k_B T$)

$$\theta \;=\; \frac{1}{3} m < |\mathbf{v} - \mathbf{u}|^2 >, \tag{32}$$

$$\mathbf{Q} \;=\; \frac{1}{2} \rho < (\mathbf{v} - \mathbf{u}) \; |\mathbf{v} - \mathbf{u}|^2 > . \tag{33}$$

Then

$$\frac{1}{2}\rho < v_i \ |\mathbf{v}-\mathbf{u}|^2 > \ = \ \frac{1}{2}\rho < (v_i - u_i) \ |\mathbf{v}-\mathbf{u}|^2 > + \frac{1}{2}\rho u_i < |\mathbf{v}-\mathbf{u}|^2 >, \qquad (34)$$

$$= \ Q_i + \frac{3}{2}(\rho \ \theta \ u_i) \quad \rightarrow \quad conduct + convect, \qquad (35)$$

and using $\rho < v_k \partial(|\mathbf{v}-\mathbf{u}|^2)/\partial x_k >= -\rho < v_k \sum_i (v_i - u_i) > \partial u_i/\partial x_k$ and

$$\rho < v_k \ (v_i - u_i) > \ = \ \rho < (v_k - u_k)(v_i - u_i) > + \rho u_k < v_i - u_i >, \qquad (36)$$

$$= \ P_{ki}, \qquad (37)$$

find

$$\frac{3}{2}\frac{\partial}{\partial t}(\rho \ \theta) + \frac{3}{2}\nabla \cdot (\rho \ \theta \ \mathbf{u}) + \nabla \cdot \mathbf{Q} + m \sum_k \sum_i P_{ki} \frac{\partial u_i}{\partial x_k} = 0. \qquad (38)$$

A final definition

$$M_{ik} = \frac{m}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right), \qquad (39)$$

use of Eq. (23) again and we have

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\theta = -\frac{2}{3}\nabla\cdot\mathbf{Q} - \frac{2}{3}\sum_k \sum_i P_{kj} M_{jk} = 0. \qquad (40)$$

F. Collect and Interpret.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \qquad (41)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)u_i \ = \ \frac{1}{m}F_i - \sum_k \frac{1}{\rho}\frac{\partial P_{ik}}{\partial x_k}, \qquad (42)$$

$$= \ external\ force \ + \ internal\ force. \qquad (43)$$

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla\right)\theta \ = \ -\frac{2}{3}\nabla\cdot\mathbf{Q} - \frac{2}{3}\sum_k \sum_i P_{kj} M_{jk} = 0, \qquad (44)$$

$$= \ conduction \ + \ internal\ work. \qquad (45)$$

Definitions:

$$n(\mathbf{x},t) = \int d\mathbf{p}\; f(\mathbf{x},\mathbf{p},t), \tag{46}$$

$$< \cdots (\mathbf{x},t) > = \frac{1}{n}\int d\mathbf{p}\; \cdots\; f(\mathbf{x},\mathbf{p},t), \tag{47}$$

$$\rho(\mathbf{x},t) = mn, \tag{48}$$

$$\mathbf{u}(\mathbf{x},t) = < \mathbf{v} >, \tag{49}$$

$$\theta(\mathbf{x},t) = \frac{1}{3} m < |\mathbf{v}-\mathbf{u}|^2 >, \tag{50}$$

$$\mathbf{Q}(\mathbf{x},t) = \frac{1}{2}\rho < (\mathbf{v}-\mathbf{u})|\mathbf{v}-\mathbf{u}|^2 >, \tag{51}$$

$$P_{ij}(\mathbf{x},t) = \rho < (v_i - u_i)(v_j - u_j) >, \tag{52}$$

$$M_{ik}(\mathbf{x},t) = \frac{m}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right). \tag{53}$$