Objectives

1. Boltzmann H-theorem.
2. Normal solution $f^{(0)}$.
3. Calculation of mass flux, pressure tensor as well as heat flux using $f^{(0)}$.

Rewriting again for the Boltzmann Equation, we get:

$$\frac{\partial f_j}{\partial t} + \mathbf{v_j} \cdot \nabla_{\mathbf{r}} f_j + \frac{\mathbf{F_j}}{m_j} \cdot \nabla_{\mathbf{v}} f_j = 2\pi \sum_i \int_{-\infty}^{\infty} \int_0^{\infty} \left(f_i' f_j' - f_i f_j \right) v_r b db d\mathbf{v_i} \tag{1}$$

Now consider the phase space distribution of all particles, which are identical to one another such that we have a one-component system. In this case, we can drop the summation operator $\sum_i$ and all the subscripts j and change the subscript i to 1, such that we have:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \frac{\mathbf{F}}{m} \cdot \nabla_{\mathbf{v}} f = 2\pi \int_{-\infty}^{\infty} \int_0^{\infty} \left(f_1' f' - f_1 f \right) v_r b db d\mathbf{v_1} \tag{2}$$

We then write the following H function:

$$H(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f \ln f d\mathbf{r} d\mathbf{v} \tag{3}$$

Taking time derivative of both sides:

$$\frac{dH(t)}{dt} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Big(\ln f\frac{\partial f}{\partial t} + \frac{\partial f}{\partial t}\Big)d\mathbf{r}d\mathbf{v} \tag{4}$$

As total number of points in phase space does not change with time, we can write:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial f}{\partial t}d\mathbf{r}d\mathbf{v} = \frac{\partial}{\partial t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}fd\mathbf{r}d\mathbf{v} = 0 \tag{5}$$

We know that:

$$\begin{aligned}&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\ln f)\mathbf{v}\cdot\nabla_{\mathbf{r}}fd\mathbf{r}d\mathbf{dv}\\ &= \sum_{k=x,y,z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}v_k(\ln f)\frac{\partial}{\partial k}fdkdv_k\\ &= \sum_{k=x,y,z}\int_{-\infty}^{\infty}v_k\Big[f\ln f|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}df\Big]dv_k = 0\end{aligned}$$

Similarly, we also know that:

$$\begin{aligned}
&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(\ln f)\frac{\mathbf{F}}{m}\cdot\nabla_{\mathbf{v}} f d\mathbf{r}d\mathbf{dv} \\
&=\sum_{k=x,y,z}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{F_k}{m}(\ln f)\frac{\partial}{\partial v_k} f dk dv_k \\
&=\sum_{k=x,y,z}\int_{-\infty}^{\infty}\frac{F_k}{m}\left[f\ln f\Big|_{-\infty}^{\infty}-\int_{-\infty}^{\infty}df\right]dk=0
\end{aligned}$$

With these, we can write:

$$\frac{dH(t)}{dt}=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left[2\pi(\ln f)\int_{-\infty}^{\infty}\int_{0}^{\infty}(f_1'f'-f_1f)v_r b db d\mathbf{v_1}\right]d\mathbf{r}d\mathbf{v} \tag{6}$$

Looking at the collision integral more carefully, we find that:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln f)(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$
$$= -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln f')(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$

Then we have:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln f)(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$
$$= \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln \frac{f}{f'})(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$

Similarly for f_1:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln f_1)(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$
$$= \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln \frac{f_1}{f_1'})(f_1'f' - f_1 f)v_r b db d\mathbf{v_1} d\mathbf{r} d\mathbf{v}$$

As we only have one component and the collision is elastic, an interchange of the f and f_1 is not going to affect the value of the integral, we then have:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\ln f)(f_1'f' - f_1 f)v_r bdbd\mathbf{v_1}d\mathbf{r}d\mathbf{v}$$
$$= \frac{1}{4}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\ln\left(\frac{f_1 f}{f_1' f'}\right)(f_1'f' - f_1 f)v_r bdbd\mathbf{v_1}d\mathbf{r}d\mathbf{v}$$

At equilibrium, $dH(t)/dt = 0$. This suggests that:

$$\frac{f'f_1' - ff_1}{4}\ln\left(\frac{ff_1}{f'f_1'}\right) = 0 \tag{7}$$

$$\ln f + \ln f_1 = \ln f' + \ln f_1' \tag{8}$$

This bears a close resemblance with conservation law, which leads to the result that $\ln f$ should be a linear combination of m, $m\mathbf{v}$ and $\frac{1}{2}mv^2$ as these quantities are conserved.

$$\ln f = c_1 m + m\mathbf{c_2} \cdot \mathbf{v} - \frac{c_3}{2} m v^2 \tag{9}$$

c_1, $\mathbf{c_2}$ and c_3 are constants. f should have the following form:

$$f = c \exp\big[- \frac{c_3}{2} m (\mathbf{v} - \frac{\mathbf{c_2}}{c_3})^2 \big] \tag{10}$$

where $c = \exp[c_1 m + m c_2^2/(2c_3)]$. These constants can be found as follows:

$$\rho = \int_{-\infty}^{\infty} f d\mathbf{v} \tag{11}$$

$$c = \left(\frac{c_3 m}{2\pi} \right)^{1.5} \rho(\mathbf{r}, t) \tag{12}$$

$$\mathbf{v_0} = \frac{1}{\rho}\int_{-\infty}^{\infty} \mathbf{v} f d\mathbf{v}$$
$$= \int_{-\infty}^{\infty} \mathbf{v}(\frac{c_3 m}{2\pi})^{1.5} \exp\Big[-\frac{c_3}{2}m(\mathbf{v}-\frac{\mathbf{c_2}}{c_3})^2\Big]d\mathbf{v}$$
$$= \frac{\mathbf{c_2}}{c_3}$$

$$(\mathbf{v}-\mathbf{v_0})^2 = \int_{-\infty}^{\infty}(\mathbf{v}-\mathbf{v_0})^2\Big(\frac{c_3 m}{2\pi}\Big)^{1.5}\exp[-\frac{c_3}{2}m(\mathbf{v}-\mathbf{v_0})^2]d\mathbf{v}$$
$$= \int_0^{\infty} 4\pi\Big(\frac{c_3 m}{2\pi}\Big)^{1.5}(v-v_0)^4\exp\Big[-\frac{c_3 m}{2}(\mathbf{v}-\mathbf{v_0})^2\Big]d(v-v_0)$$
$$= \frac{3}{c_3 m}$$

As we know that $\frac{m(\mathbf{v}-\mathbf{v_0})^2}{2} = \frac{3k_bT}{2}$, $c_3 = \frac{1}{k_bT}$.

This implies:

$$f = \rho(\mathbf{r}, t)\Big(\frac{m}{2\pi k_b T(\mathbf{r}, t)}\Big)^{1.5} \exp\Big[-\frac{m(\mathbf{v} - \mathbf{v_0}(\mathbf{r}, t))^2}{2k_b T(\mathbf{r}, t)}\Big] \qquad (13)$$

Note that we have dropped the subscript j for convenience. For mass flux, we have:

$$\mathbf{J} = \rho m \langle(\mathbf{v} - \mathbf{v_0})\rangle = m\int_{-\infty}^{\infty} (\mathbf{v} - \mathbf{v_0}) f d\mathbf{v} = \mathbf{0}$$

$$\mathsf{P} = \rho m \langle(\mathbf{v} - \mathbf{v_0})(\mathbf{v} - \mathbf{v_0})\rangle$$

$$p_{xy} = m\int_{-\infty}^{\infty} (v_x - v_{0,x})(v_y - v_{0,y}) f d(\mathbf{v} - \mathbf{v_0}) = \rho m \langle c_x c_y\rangle = 0$$

$$p_{xx} = \rho m \langle c_x^2\rangle = \frac{\rho}{2b} = \rho k_b T$$

For which we have let $\mathbf{c} = (\mathbf{v} - \mathbf{v_0})$.

$$\mathbf{q} = \frac{m}{2}\int_{-\infty}^{\infty} c^2 \mathbf{c} f d\mathbf{c}$$

$$q_x = \frac{\rho m}{2}\int_0^{2\pi} \cos^3\psi d\psi \int_0^{\pi} \sin^4\theta d\theta \int_0^{\infty} c^5 \left(\frac{b}{\pi}\right)^{1.5} e^{-bc^2} dc$$

This is because $c_x = c\sin\theta\cos\psi$. Easiest integral to evaluate is:

$$\begin{aligned}\int_0^{2\pi} \cos^3\psi d\psi &= \int_0^{2\pi} (1-\sin^2\psi)\cos\psi d\psi \\ &= \int_0^{0} (1-\sin^2\psi) d\sin\psi = 0\end{aligned}$$

Similarly, $q_y = 0$ as $c_y = c\cos\theta\sin\psi$. $q_z = 0$, as the integral for ψ is:

$$\int_0^{2\pi} \sin^3\psi d\psi = \int_0^{2\pi} (1-\cos^2\psi)\sin\psi d\psi = \int_1^{1} (\cos^2\psi - 1) d\cos\psi = 0$$