Kinetic Theory

1. *Poisson Brackets:*

(a) Show that for observable $\mathcal{O}(\mathbf{p}(\mu), \mathbf{q}(\mu))$, $d\mathcal{O}/dt = \{\mathcal{O}, \mathcal{H}\}$, along the time trajectory of any micro state μ, where $\mathcal{H}$ is the Hamiltonian.

• Following the trajectory of each micro state, we find

$$\frac{d\mathcal{O}(\mathbf{p},\mathbf{q})}{dt} = \sum_{\alpha=1}^{3N}\left(\frac{\partial \mathcal{O}}{\partial p_\alpha}\cdot\frac{\partial p_\alpha}{\partial t} + \frac{\partial \mathcal{O}}{\partial q_\alpha}\cdot\frac{\partial q_\alpha}{\partial t}\right) = -\sum_{\alpha=1}^{3N}\left(\frac{\partial \mathcal{O}}{\partial p_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial q_\alpha} - \frac{\partial \mathcal{O}}{\partial q_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial p_\alpha}\right) = \{\mathcal{O},\mathcal{H}\}.$$

(b) If the ensemble average $\langle\{\mathcal{O}, \mathcal{H}\}\rangle = 0$ for any observable $\mathcal{O}(\mathbf{p}, \mathbf{q})$ in phase space, show that the ensemble density satisfies $\{\mathcal{H}, \rho\} = 0$.

• The ensemble average of the Poisson bracket is

$$\langle\{\mathcal{O},\mathcal{H}\}\rangle = -\sum_{\alpha=1}^{3N}\int d\Gamma\rho\left[\left(\frac{\partial \mathcal{O}}{\partial p_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial q_\alpha} - \frac{\partial \mathcal{O}}{\partial q_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial p_\alpha}\right)\right].$$

Integrating by parts to remove the derivatives on $\mathcal{O}$ leads to

$$\begin{aligned}\langle\{\mathcal{O},\mathcal{H}\}\rangle =& \sum_{\alpha=1}^{3N}\int d\Gamma\mathcal{O}\left[\left(\frac{\partial \rho}{\partial p_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial q_\alpha} - \frac{\partial \rho}{\partial q_\alpha}\cdot\frac{\partial \mathcal{H}}{\partial p_\alpha}\right) + \rho\left(\frac{\partial^2 \mathcal{H}}{\partial p_\alpha\partial q_\alpha} - \frac{\partial^2 \mathcal{H}}{\partial q_\alpha\partial p_\alpha}\right)\right]\\ =& \int d\Gamma\mathcal{O}\{\mathcal{H},\rho\}.\end{aligned}$$

For the integral to be zero for any choice of $\mathcal{O}(\mathbf{p}, \mathbf{q})$, we must have $\{\mathcal{H}, \rho\} = 0$.

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2. *Equilibrium density:* Consider a gas of N particles of mass m, in an external potential $U(\vec{q})$. Assume that the one body density $\rho_1(\vec{p}, \vec{q}, t)$, satisfies the Boltzmann equation. For a stationary solution, $\partial\rho_1/\partial t = 0$, it is *sufficient* from Liouville's theorem for ρ_1 to satisfy $\rho_1 \propto \exp\left[-\beta\left(p^2/2m + U(\vec{q})\right)\right]$. Prove that this condition is also *necessary* by using the H-theorem as follows.

(a) Find $\rho_1(\vec{p}, \vec{q})$ that minimizes $\mathrm{H} = N\int d^3\vec{p}d^3\vec{q}\rho_1(\vec{p}, \vec{q})\ln\rho_1(\vec{p}, \vec{q})$, subject to the constraint that the total energy $E = \langle\mathcal{H}\rangle$ is constant. (Hint: Use the method of Lagrange multipliers to impose the constraint.)

• Using Lagrange multipliers to impose the constraints, $\langle\mathcal{H}\rangle = E$ and $\int d^3\vec{p}d^3\vec{q}\,\rho_1 = 1$, minimizing H with the given constraints reduces to minimizing,

$$N\int d^3\vec{p}d^3\vec{q}(\rho_1\ln\rho_1 + \beta\rho_1\mathcal{H} + \alpha\rho_1) - \beta E - \alpha N.$$

Differentiating with respect to α, β, and the function ρ_1 we get,

$$\begin{aligned}
N\int d^3\vec{p}d^3\vec{q}\,\rho_1 = N \quad &\rightarrow \quad \int d^3\vec{p}d^3\vec{q}\,\rho_1 = 1,\\
N\int d^3\vec{p}d^3\vec{q}\,\rho_1\mathcal{H} = E \quad &\rightarrow \quad \int d^3\vec{p}d^3\vec{q}\,\rho_1\mathcal{H} = E/N,\\
\ln\rho_1 + \beta\mathcal{H} + \alpha = 0 \quad &\rightarrow \quad \rho_1 = \exp(-\beta\mathcal{H} - \alpha),
\end{aligned}$$

respectively. Hence we conclude,

$$\rho_1 = \frac{\exp(-\beta\mathcal{H})}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H})},$$

where β is determined by,

$$\frac{\int d^3\vec{p}d^3\vec{q}\,\mathcal{H}\exp(-\beta\mathcal{H})}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H})} = \frac{E}{N}.$$

(b) For a mixture of two gases (particles of masses m_a and m_b) find the distributions $\rho_1^{(a)}$ and $\rho_1^{(b)}$ that minimize $\mathrm{H} = \mathrm{H}^{(a)} + \mathrm{H}^{(b)}$ subject to the constraint of constant total energy. Hence show that the kinetic energy per particle can serve as an empirical temperature.

• If we have N_a and N_b of each particle type with total energy E, then H is minimized with the total energy constraint by extremizing,

$$\begin{aligned}
\int d^3\vec{p}d^3\vec{q}(N_a\rho_1^{(a)}\ln\rho_1^{(a)} + N_b\rho_1^{(b)}\ln\rho_1^{(b)} + \beta(N_a\mathcal{H}_a\rho_1^{(a)} + N_b\mathcal{H}_b\rho_1^{(b)})\\
+N_a\alpha\rho_1^{(a)} + N_b\alpha'\rho_1^{(b)}) - \beta E - \alpha N_a - \alpha' N_b
\end{aligned}.$$

Differentiating this expression with respect to α, α', $\beta, \rho_1^{(a)}$, and $\rho_1^{(b)}$, we get,

$$\begin{aligned}
\int d^3\vec{p}d^3\vec{q}\,\rho_1^{(a)} &= 1,\\
\int d^3\vec{p}d^3\vec{q}\,\rho_1^{(b)} &= 1,\\
\int d^3\vec{p}d^3\vec{q}\left(N_a\mathcal{H}_a\rho_1^{(a)} + N_b\mathcal{H}_b\rho_1^{(b)}\right) &= E,\\
\ln\rho_1^{(a)} + \beta\mathcal{H}_a + \alpha &= 0,\\
\ln\rho_1^{(b)} + \beta\mathcal{H}_b + \alpha' &= 0.
\end{aligned}$$

So we get,

$$\rho_1^{(a)} = \frac{\exp(-\beta\mathcal{H}_a)}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H}_a)},$$
$$\rho_2^{(a)} = \frac{\exp(-\beta\mathcal{H}_b)}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H}_b)}.$$

where β is obtained by,

$$N_a\frac{\int d^3\vec{p}d^3\vec{q}\mathcal{H}_a\exp(-\beta\mathcal{H}_a)}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H}_a)} + N_b\frac{\int d^3\vec{p}d^3\vec{q}\mathcal{H}_b\exp(-\beta\mathcal{H}_b)}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H}_b)} = E.$$

Note that β is a value defined for both gases a and b, and hence can serve as an empirical temperature.

For the specific case of

$$\mathcal{H}_a = \frac{p^2}{2m_a} + U_a(\vec{q}), \quad \mathcal{H}_b = \frac{p^2}{2m_a} + U_b(\vec{q}),$$

the kinetic energy per particle in a distribution with equal β is also equal, since

$$\begin{aligned}
\frac{\int d^3\vec{p}d^3\vec{q}\frac{p^2}{2m_a}\exp\left[-\beta(p^2/2m_a + U_a(\vec{q}))\right]}{\int d^3\vec{p}d^3\vec{q}\exp(-\beta\mathcal{H}_a)} &= \frac{\int d^3\vec{q}\exp(-\beta U_a)\int d^3\vec{p}\frac{p^2}{2m_a}\exp(-\beta p^2/2m_a)}{\int d^3\vec{q}\exp(-\beta U_a)\int d^3\vec{p}\exp(-\beta p^2/2m_a)} \\
&= \frac{4\pi\int_0^\infty dp\frac{p^4}{2m_a}\exp(-\beta p^2/2m_a)}{4\pi\int_0^\infty dp\, p^2\exp(-\beta p^2/2m_a)} \\
&= \frac{1}{\beta}\frac{\int_0^\infty dt\, t^4 e^{-t^2}}{\int_0^\infty dt\, t^2 e^{-t^2}} = \frac{3}{2\beta}
\end{aligned}.$$

So we see that the kinetic energy per particle for the gas can also serve as an empirical temperature in this case.

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3. (Optional) *Evolving a canonical harmonic oscillator density:* A dilute gas of non-interacting particles is in equilibrium in a harmonic potential, such that the density for each particle has the form

$$\rho_0(\vec{q},\vec{p}) = \exp\left[-\beta\left(\frac{Kq^2}{2} + \frac{p^2}{2m}\right)\right]\left(\frac{\beta}{2\pi}\right)^3\left(\frac{K}{m}\right)^{3/2}.$$

At time $t = 0$, and external force $\vec{F}(t)$ is applied, changing the one particle Hamiltonian to $H_0 - \vec{q}\cdot\vec{F}(t)$.

(a) Write down the (Liouville) equation governing subsequent evolution of the one particle density.

•

$$\frac{\partial \rho}{\partial t} = \left\{ \frac{Kq^2}{2} + \frac{p^2}{2m} - \vec{q} \cdot \vec{F}(t), \rho \right\} = \left(K\vec{q} - \vec{F} \right) \cdot \frac{\partial \rho}{\partial \vec{p}} - \frac{\vec{p}}{m} \cdot \frac{\partial \rho}{\partial \vec{q}} .$$

(b) Confirm that the density at later times satisfies, $\rho(\vec{q}, \vec{p}, t) = \rho_0 \left(\vec{q} - \langle \vec{q} \rangle_t, \vec{p} - \langle \vec{p} \rangle_t \right)$, and find the equations of motion for $\langle \vec{q} \rangle_t$ and $\langle \vec{p} \rangle_t$.

• Dividing by $\beta\rho$, we note that the equation of motion is the same for the proposed solution

$$-\frac{\ln \rho}{\beta} = \frac{K \left(\vec{q} - \langle \vec{q} \rangle_t \right)^2}{2} + \frac{\left(\vec{p} - \langle \vec{p} \rangle_t \right)^2}{2m} - \frac{3}{\beta} \ln \left(\frac{\beta}{2\pi} \sqrt{\frac{K}{m}} \right) .$$

It is now easy to check that

$$\begin{aligned} \frac{1}{\beta} \frac{\partial \ln \rho}{\partial t} &= K \left(\vec{q} - \langle \vec{q} \rangle_t \right) \cdot \frac{d \langle \vec{q} \rangle_t}{dt} + \frac{1}{m} \left(\vec{p} - \langle \vec{p}, \rangle_t \right) \cdot \frac{d \langle \vec{p} \rangle_t}{dt} \\ \frac{1}{\beta} \frac{\partial \ln \rho}{\partial \vec{p}} &= -\frac{1}{m} \left(\vec{p} - \langle \vec{p} \rangle_t \right) \\ \frac{1}{\beta} \frac{\partial \ln \rho}{\partial \vec{q}} &= -K \left(\vec{q} - \langle \vec{q} \rangle_t \right) \end{aligned} .$$

To satisfy the Liouville equation, we must have

$$K \left(\vec{q} - \langle \vec{q} \rangle_t \right) \cdot \frac{d \langle \vec{q} \rangle_t}{dt} + \frac{1}{m} \left(\vec{p} - \langle \vec{p}, \rangle_t \right) \cdot \frac{d \langle \vec{p} \rangle_t}{dt} = -\left(K\vec{q} - \vec{F} \right) \cdot \left(\frac{\vec{p} - \langle \vec{p} \rangle_t}{m} \right) + \frac{K\vec{p}}{m} \cdot \left(\vec{q} - \langle \vec{q} \rangle_t \right) .$$

There are 4 types of terms in the above equation: *(i)* Two terms proportional to $\vec{p} \cdot \vec{q}$ on the right hand side simply cancel out; *(ii)* Terms proportional to $\vec{q}$ lead to the evolution equation

$$\frac{d \langle \vec{q} \rangle_t}{dt} = \frac{\langle \vec{p} \rangle_t}{m} ;$$

(iii) Terms proportional to $\vec{p}$ lead to the evolution equation

$$\frac{d \langle \vec{p} \rangle_t}{dt} = -K \langle \vec{q} \rangle_t + \vec{F}(t) ;$$

(iv) The constant terms can be organized as

$$K \langle \vec{q} \rangle_t \cdot \frac{d \langle \vec{q} \rangle_t}{dt} + \frac{1}{m} \langle \vec{p}, \rangle_t \cdot \frac{d \langle \vec{p} \rangle_t}{dt} = -\frac{1}{m} \vec{F} \cdot \langle \vec{p} \rangle_t ,$$

which is consistent with the two equations of motion, and an expression of conservation of energy. Hence, we observe that the proposed ρ, with shifted averages for position and momentum, satisfies the Liouville equation, as long as the two averages satisfy the Hamiltonian equations of motion in the presence of the external force.

(c) Compute the entropy $S(t)$ associated with the probability density ρ.

• The entropy for the time dependent Gaussain probability distribution takes the form

$$S(t) = -\int d^3\vec{p}d^3\vec{q}\,\rho\ln\rho = \left\langle \frac{\beta K\left(\vec{q}-\langle\vec{q}\rangle_t\right)^2}{2} + \frac{\beta\left(\vec{p}-\langle\vec{p}\rangle_t\right)^2}{2m} - 3\ln\left(\frac{\beta}{2\pi}\sqrt{\frac{K}{m}}\right)\right\rangle .$$

The averages are taken with the Gaussian distribution; each quadratic term contributing a factor of 1/2. Noting that the vectors $\vec{q}$ and $\vec{p}$ have three components each, we conclude

$$S(t) = 3 - 3\ln\left(\frac{\beta}{2\pi}\sqrt{\frac{K}{m}}\right) .$$

This result provides an explanation of why the inverse temperature β is not changed during the process: Liouville's equation preserves the entropy, which for a Gaussian distribution only the depends on the variance.

(d) Would a similar time dependent shift of the density work in the case of the canonical weight associated with a general potential $\mathcal{V}(\vec{q})$ (e.g.$\mathcal{V}(\vec{q}) \propto q^4$) driven by an external force?

• No, in general it is not possible to satisfy the Lioville equation by a shift of arguments in the canonical density. The Harmonic oscillator is special in that the linear equations of motion map the Gaussian density of states to another Gaussian.

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4. *Zeroth-order hydrodynamics:* The hydrodynamic equations resulting from the conservation of particle number, momentum, and energy in collisions are (in a uniform box):

$$\begin{cases} \partial_t n + \partial_\alpha\left(nu_\alpha\right) = 0 \\ \partial_t u_\alpha + u_\beta\partial_\beta u_\alpha = -\dfrac{1}{mn}\partial_\beta P_{\alpha\beta} \\ \partial_t\varepsilon + u_\alpha\partial_\alpha\varepsilon = -\dfrac{1}{n}\partial_\alpha h_\alpha - \dfrac{1}{n}P_{\alpha\beta}u_{\alpha\beta} \end{cases} ,$$

where n is the local density, $\vec{u} = \langle\vec{p}/m\rangle$, $u_{\alpha\beta} = \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right)/2$, and $\varepsilon = \left\langle mc^2/2\right\rangle$, with $\vec{c} = \vec{p}/m - \vec{u}$.

(a) For the zeroth order density

$$f_1^0(\vec{p},\vec{q},t) = \frac{n(\vec{q},t)}{\left(2\pi m k_B T(\vec{q},t)\right)^{3/2}} \exp\left[-\frac{\left(\vec{p}-m\vec{u}(\vec{q},t)\right)^2}{2mk_B T(\vec{q},t)}\right],$$

calculate the pressure tensor $P^0_{\alpha\beta} = mn\left\langle c_\alpha c_\beta\right\rangle^0$, and the heat flux $h^0_\alpha = nm\left\langle c_\alpha c^2/2\right\rangle^0$.

• The PDF for $\vec{c}$ is proportional to the Gaussian $\exp\left(-mc^2/(2k_BT)\right)$, from which we immediately get

$$\left\langle c_\alpha c_\beta\right\rangle^0 = \frac{k_BT}{m}\delta_{\alpha\beta} \quad\Longrightarrow\quad P^0_{\alpha\beta} = nk_BT\delta_{\alpha\beta}, \quad \text{and} \quad \varepsilon = \frac{3}{2}k_BT.$$

All odd expectation values of the symmetric weight are zero, specifically $\langle\vec{c}\rangle = 0$, and $\left\langle\vec{h}^0\right\rangle = 0$.

(b) Obtain the zeroth order hydrodynamic equations governing the evolution of $n(\vec{q},t)$, $\vec{u}(\vec{q},t)$, and $T(\vec{q},t)$.

• Substituting $P^0_{\alpha\beta} = nk_BT\delta_{\alpha\beta}$, $\varepsilon = 3k_BT/2$, and $\left\langle\vec{h}^0\right\rangle = 0$ in the hydrodynamic equations gives:

$$\begin{cases} \partial_t n + u_\alpha\partial_\alpha n = -n\partial_\alpha u_\alpha \\ \partial_t u_\alpha + u_\beta\partial_\beta u_\alpha = -\dfrac{k_B}{mn}\partial_\alpha(nT) \\ \dfrac{3}{2}\left(\partial_t T + u_\alpha\partial_\alpha T\right) = -T\partial_\alpha u_\alpha \end{cases}.$$

(c) Show that the above equations imply $D_t\ln\left(nT^{-3/2}\right) = 0$, where $D_t = \partial_t + u_\beta\partial_\beta$ is the material derivative along streamlines.

• Using $D_t = \partial_t + u_\beta\partial_\beta$, the above equations can be written as

$$\begin{cases} D_t\ln n = -\partial_\alpha u_\alpha \\ D_t u_\alpha = -\dfrac{k_B}{mn}\partial_\alpha(nT) \\ \dfrac{3}{2}D_t\ln T = -\partial_\alpha u_\alpha \end{cases}.$$

Eliminating $\partial_\alpha u_\alpha$ between the first and third equations gives the required result of $D_t\ln\left(nT^{-3/2}\right) = 0$.

(d) Write down the expression for the function $\mathrm{H}^0(t) = \int d^3\vec{q}d^3\vec{p}f_1^0(\vec{p},\vec{q},t)\ln f_1^0(\vec{p},\vec{q},t)$, after performing the integrations over $\vec{p}$, in terms of $n(\vec{q},t)$, $\vec{u}(\vec{q},t)$, and $T(\vec{q},t)$.

• Using the expression for f_1^0,

$$\mathrm{H}^0(t) = \int d^3\vec{q} d^3\vec{p} \frac{n}{(2\pi m k_B T)^{3/2}} \exp\left[-\frac{(\vec{p}-m\vec{u})^2}{2mk_BT}\right] \times \left[\ln\left(nT^{-3/2}\right) - \frac{3}{2}\ln\left(2\pi m k_B\right) - \frac{(\vec{p}-m\vec{u})^2}{2mk_BT}\right].$$

The Gaussian averages over $\vec{p}$ are easily performed to yield

$$\mathrm{H}^0(t) = \int d^3\vec{q} n \left[\ln\left(nT^{-3/2}\right) - \frac{3}{2}\ln\left(2\pi m k_B\right) - \frac{3}{2}\right].$$

(e) Using the hydrodynamic equations in (b) calculate $d\mathrm{H}^0/dt$.

• Taking the time derivative inside the integral gives

$$\frac{d\mathrm{H}^0}{dt} = \int d^3\vec{q} \left[\partial_t n \ln\left(nT^{-3/2}\right) + n\partial_t \ln\left(nT^{-3/2}\right)\right].$$

Use the results of parts (b) and (c) to substitute for $\partial_t n$ and $\partial_t \ln\left(nT^{-3/2}\right)$, to get

$$\begin{aligned}\frac{d\mathrm{H}^0}{dt} &= -\int d^3\vec{q} \left[\ln\left(nT^{-3/2}\right)\partial_\alpha\left(nu_\alpha\right) + nu_\alpha\partial_\alpha \ln\left(nT^{-3/2}\right)\right] \\ &= -\int d^3\vec{q}\,\partial_\alpha\left[nu_\alpha \ln\left(nT^{-3/2}\right)\right] = 0,\end{aligned}$$

since the integral of a complete derivative is zero.

(f) Discuss the implications of the result in (e) for approach to equilibrium.

• The expression for $-\mathrm{H}^0$ is related to the entropy of the gas. The result in (f) implies that the entropy of the gas does not change if its n $\vec{u}$, and T vary according to the zeroth order equations. The corrections due to first order hydrodynamics are necessary in order to describe the increase in entropy.

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5. *Diffusion:* Consider a mixture of two gases (a) and (b), in a box of volume V.

(a) Write down the Boltzmann equations for the one particle densities f_a, and, f_b, in terms of the Liouville operators $\mathcal{L}_\alpha \equiv [\partial_t + (\vec{p}_\alpha/m_\alpha)\cdot\nabla]$, and collision operators

$$C_{\alpha,\beta} = -\int d^3\vec{p}_2 d^2\vec{b}_{\alpha\beta}\ |\vec{v}_1 - \vec{v}_2|\left[f_\alpha(\vec{p}_1,\vec{q}_1)f_\beta(\vec{p}_2,\vec{q}_1) - f_\alpha(\vec{p}_1{}',\vec{q}_1)f_\beta(\vec{p}_2{}',\vec{q}_1)\right],$$

where $\alpha = a, b$ and $\beta = a, b$.

• The Boltzmann equation for one type of gas is easily generalized to two as

$$\begin{cases} \mathcal{L}_a f_a = C_{a,a} + C_{a,b} \\ \mathcal{L}_b f_b = C_{b,a} + C_{b,b} \end{cases} .$$

(b) Assuming that the collision terms are much more dominant than the Liouville streams (dilute limit), write down a zeroth order solution to the Boltzmann equations.

• The collision terms $C_{a,a}$ and $C_{b,b}$ are the same as for one type of particle, and are set to zero is $\ln f_\alpha = a_\alpha + \vec{b}_\alpha \cdot \vec{p} + \beta_\alpha p^2/(2m_x)$ for $\alpha = a, b$, since particle number, momentum, and energy are conserved in the collision. To set $C_{a,b} = 0$, we then need $\vec{b}_a = \vec{b}_b$ and $\beta_a = \beta_b$ for each $\vec{q}$ and t. After exponentiation, the zeroth order solutions can be cast as

$$\begin{cases} f_a^0(\vec{q}, \vec{p}, t) = n_a(\vec{q}, t) \left(\dfrac{\beta(\vec{q}, t)}{2\pi m_a} \right)^{3/2} \exp\left[-\dfrac{\beta(\vec{q}, t)(\vec{p} - m_a \vec{u}(\vec{q}, t))^2}{2m_a} \right] \\ f_b^0(\vec{q}, \vec{p}, t) = n_b(\vec{q}, t) \left(\dfrac{\beta(\vec{q}, t)}{2\pi m_b} \right)^{3/2} \exp\left[-\dfrac{\beta(\vec{q}, t)(\vec{p} - m_b \vec{u}(\vec{q}, t))^2}{2m_b} \right] \end{cases} .$$

(c) Write down the hydrodynamic equations governing $n_a(\vec{q}, t)$ and $n_b(\vec{q}, t)$.

• The continuity of particle number leads to

$$\partial_t n_\alpha + \nabla \left(n_\alpha \vec{u}_\alpha \right) = 0, \quad \text{for} \quad \alpha = a, b \,,$$

where $\vec{u}_\alpha = \langle \vec{p}_\alpha / m_\alpha \rangle$.

(d) Write down the one particle densities corresponding to a configuration in which $n_a(\vec{q}) + n_b(\vec{q}) = n$ is uniform across a system at rest and at uniform temperature, i.e. $\vec{u} = 0$ with n and T constant throughout. Does a non-uniform mixture, with spatially varying $n_a(\vec{q})$ and $n_b(\vec{q})$, come to equilibrium in zeroth order hydrodynamics?

• Adapting the more general result to this configuration, gives

$$\begin{cases} f_a^0(\vec{q}, \vec{p}) = n_a(\vec{q}) \left(\dfrac{\beta}{2\pi m_a} \right)^{3/2} \exp\left[-\dfrac{\beta \vec{p}^{\,2}}{2m_a} \right] \\ f_b^0(\vec{q}, \vec{p}) = n_b(\vec{q}) \left(\dfrac{\beta}{2\pi m_b} \right)^{3/2} \exp\left[-\dfrac{\beta \vec{p}^{\,2}}{2m_b} \right] \end{cases} .$$

Since $\vec{u}_\alpha = \langle \vec{p}_\alpha / m_\alpha \rangle = 0$ for this configuration, the continuity equations imply $\partial_t n_\alpha = 0$, i.e. the densities remain inhomogeneous and do not relax to the uniform state.

(e) The first order solutions to the Boltzmann equation are given by

$$f_\alpha^1(\vec{q},\vec{p},t) = f_\alpha^0\left[1 - \tau_\alpha \mathcal{L}_\alpha[\ln f_\alpha^0]\right] ,$$

where τ_α is a characteristic time between collisions. Compute $\vec{u}_\alpha = \langle \vec{p}_\alpha/m_\alpha \rangle$ at first order.

• From $\mathcal{L}_\alpha \equiv [\partial_t + (\vec{p}_\alpha/m_\alpha)\cdot\nabla]$, and since the only variations are in $n_\alpha(\vec{q},t)$ we obtain

$$f_\alpha^1(\vec{q},\vec{p},t) = f_\alpha^0\left[1 - \tau_\alpha \frac{\partial_t n_\alpha + (\vec{p}_\alpha/m_\alpha)\cdot\nabla n_\alpha}{n_\alpha}\right] .$$

The symmetric Gaussian weight in f_α^0 now leads to the average

$$\vec{u}_\alpha = \langle \frac{\vec{p}_\alpha}{m_\alpha} \rangle = -\frac{\tau_\alpha}{m_\alpha^2 n_\alpha}\frac{m_\alpha}{\beta}\nabla n_\alpha = -\tau_\alpha \frac{k_B T}{m_\alpha}\frac{\nabla n_\alpha}{n_\alpha} .$$

(f) Show that in first order hydrodynamics the densities relax by diffusion, and identify the diffusion constant.

• The continuity equation now leads to

$$\partial_t n_\alpha = -\nabla\cdot(n_\alpha u_\alpha) = \nabla\cdot\left(\frac{\tau_\alpha k_B T}{m_\alpha}\nabla n_\alpha\right) = D_\alpha \nabla^2 n_\alpha ,$$

with $D_\alpha = \tau_\alpha k_B T/m_\alpha$.

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6. *Viscosity:* Consider a classical gas between two plates separated by a distance w. One plate at $y=0$ is stationary, while the other at $y=w$ moves with a constant velocity $v_x = u$. A zeroth order approximation to the one particle density is,

$$f_1^0(\vec{p},\vec{q}) = \frac{n}{(2\pi m k_B T)^{3/2}} \exp\left[-\frac{1}{2mk_BT}\left((p_x - m\alpha y)^2 + p_y^2 + p_z^2\right)\right] ,$$

obtained from the *uniform* Maxwell–Boltzmann distribution by substituting the average value of the velocity at each point. ($\alpha = u/w$ is the velocity gradient.)

(a) The above approximation does not satisfy the Boltzmann equation as the collision term vanishes, while $df_1^0/dt \neq 0$. Find a better approximation, $f_1^1(\vec{p})$, by linearizing the Boltzmann equation, in the single collision time approximation, to

$$\mathcal{L}\left[f_1^1\right] \approx \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m}\cdot\frac{\partial}{\partial \vec{q}}\right] f_1^0 \approx -\frac{f_1^1 - f_1^0}{\tau_\times},$$

where $\tau_\times$ is a characteristic mean time between collisions.

• We have

$$\left(\frac{\partial}{\partial t}+\frac{\vec{p}}{m}\cdot\frac{\partial}{\partial\vec{q}}\right)f_1^0=\frac{\alpha}{mk_BT}p_y(p_x-m\alpha y)f_1^0,$$

whence

$$f_1^1=f_1^0\left\{1-\tau_x\frac{\alpha}{mk_BT}p_y(p_x-m\alpha y)\right\}.$$

(b) Calculate the net transfer Π_{xy} of the x component of the momentum, of particles passing through a plane at y, per unit area and in unit time.

• The transfer of x-momentum in the y direction, across a plane at y, per unit area and per unit time, is calculated as

$$\begin{aligned}
\Pi_{xy}&=\int_{p_y>0}d^3p\frac{p_y}{m}p_xf_1^1(y)-\int_{p_y<0}d^3p\frac{(-p_y)}{m}p_xf_1^1(y)\\
&=\int d^3p\frac{p_y}{m}p_xf_1^1(y)\\
&=\int d^3p\frac{p_y}{m}p_x\left(-\frac{\tau_x\alpha}{mk_BT}\right)p_y(p_x-m\alpha y)f_1^0\\
&=-\frac{\tau_x\alpha n}{m^2k_BT}\left\{\int dp_x(p_x-m\alpha y)^2\frac{\exp\left(-\frac{(p_x-m\alpha y)^2}{2mk_BT}\right)}{\sqrt{2\pi mk_BT}}\right\}\cdot\left\{\int dp_yp_y^2\frac{\exp\left(-\frac{p_y^2}{2mk_BT}\right)}{\sqrt{2\pi mk_BT}}\right\}\\
&=-\frac{\tau_x\alpha n}{m^2k_BT}(mk_BT)^2=-\alpha n\tau_xk_BT.
\end{aligned}$$

(c) Note that the answer to (b) is independent of y, indicating a uniform transverse force $F_x=-\Pi_{xy}$, exerted by the gas on each plate. Find the coefficient of viscosity, defined by $\eta=F_x/\alpha$.

• From part (b),

$$\eta=\frac{F_x}{a}=n\tau_xk_BT.$$

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7. *Effusion:* The probability distribution for speed c of particles of mass m in a gas at temperature T is proportional to $c^2e^{-\frac{c^2}{2\sigma^2}}$, with $\sigma^2=k_BT/m$. Some particles are allowed to leak (effuse) out of a small hole with diameter much less than the mean free path.

(a) Show that the probability distribution for speed of the escaping particles is proportional to $c^3 e^{-\frac{c^2}{2\sigma^2}}$.

• The number of leaked particles with velocity $\vec{c}$ is proportional to product of finding particles of such velocity in the container, and their flux through the hole. The latter introduces a factor of $c\cos\theta$, where θ is the angle between $\vec{c}$ and the normal to the wall at position of the hole. Naturally, only positive values of $\cos\theta$ are allowed for leaking particles. Integrating over all allowed angles results in a PDF proportional to $c \times c^2 e^{-\frac{c^2}{2\sigma^2}}$, which after normalization gives

$$p(c) = \frac{c^3}{2\sigma^4} e^{-\frac{c^2}{2\sigma^2}} .$$

(b) Find the average kinetic energy of the escaping particles.

• The average kinetic energy of the leaked particles is

$$\left\langle \frac{mc^2}{2} \right\rangle = \int_0^\infty dc \frac{c^3}{2\sigma^4} e^{-\frac{c^2}{2\sigma^2}} \frac{mc^2}{2} .$$

Changing variables to $y = c^2/(2\sigma^2) = mc^2/(2k_B T)$ yields

$$\left\langle \frac{mc^2}{2} \right\rangle = k_B T \int_0^\infty dy y^2 e^{-y} = 2k_B T.$$

(c) What is the fraction of escaping particles with kinetic energy greater than $\mathcal{E}$?

• The probability density for energy is obtained from $p(E)dE = p(c)dc$ with $E = mc^2/2$. It is easy to see that this leads to $p(E) \propto E e^{-E/k_B T}$, which can be normalized to

$$p(E) = \frac{E}{(k_B T)^2} e^{-\frac{E}{k_B T}} .$$

The fraction of particles with energy $E \geq \mathcal{E}$ is now obtained from

$$\overline{P}(\mathcal{E}) = \int_{\mathcal{E}}^\infty dE p(E) = \int_{\beta\mathcal{E}}^\infty dy y e^{-y} = \left(1 + \frac{\mathcal{E}}{k_B T}\right) e^{-\frac{\mathcal{E}}{k_B T}} .$$

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