8.333: Statistical Mechanics I Problem Set # **3** Due: **10/25/2021**

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.

(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 $\{\mathcal{H}, \rho\} = 0$.

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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.)

(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.

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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.

(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 $\langle\vec{p}\rangle_t$.

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

(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?

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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

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

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

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

(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.

(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 $T(\vec{q},t)$.

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

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

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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 $\beta = a, b$.

(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.

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

(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?

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

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

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

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

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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,

$$f^0_1(\vec{p},\vec{q}) = \frac{n}{(2\pi m k_B T)^{3/2}} \exp\left[-\frac{1}{2mk_BT}\left((p_x - m\alpha y)^2 + p_y^2 + p_z^2\right)\right],$$

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 $df^0_1/dt \neq 0$. Find a better approximation, $f^1_1(\vec{p})$, by linearizing the Boltzmann equation, in the single collision time approximation, to

$$\mathcal{L}\left[f^1_1\right] \approx \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m}\cdot\frac{\partial}{\partial \vec{q}}\right] f^0_1 \approx -\frac{f^1_1 - f^0_1}{\tau_\times},$$

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

(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.

(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 $\eta = F_x/\alpha$.

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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 $c^2 e^{-\frac{c^2}{2\sigma^2}}$, with $\sigma^2 = k_B T/m$. 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 $c^3 e^{-\frac{c^2}{2\sigma^2}}$.

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

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

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† Reviewing the problems and solutions provided on the course web-page for preparation for *Test 2* should help you with the above problems.