
Review Problems

The second in-class test will take place on Wednesday **10/24/07** from **2:30 to 4:00** pm. There will be a recitation with test review on Monday **10/22/07**.

The test is ‘closed book,’ and composed entirely from a subset of the following problems. Thus if you are familiar and comfortable with these problems, there will be no surprises!

You may find the following information helpful:

Physical Constants

Electron mass	$m_e \approx 9.1 \times 10^{-31} kg$	Proton mass	$m_p \approx 1.7 \times 10^{-27} kg$
Electron Charge	$e \approx 1.6 \times 10^{-19} C$	Planck’s const./ 2π	$\hbar \approx 1.1 \times 10^{-34} Js^{-1}$
Speed of light	$c \approx 3.0 \times 10^8 ms^{-1}$	Stefan’s const.	$\sigma \approx 5.7 \times 10^{-8} Wm^{-2}K^{-4}$
Boltzmann’s const.	$k_B \approx 1.4 \times 10^{-23} JK^{-1}$	Avogadro’s number	$N_0 \approx 6.0 \times 10^{23} mol^{-1}$

Conversion Factors

$$1atm \equiv 1.0 \times 10^5 Nm^{-2} \qquad 1\text{\AA} \equiv 10^{-10}m \qquad 1eV \equiv 1.1 \times 10^4 K$$

Thermodynamics

$$dE = TdS + dW \qquad \text{For a gas: } dW = -PdV \qquad \text{For a wire: } dW = Jdx$$

Mathematical Formulas

$$\int_0^\infty dx x^n e^{-\alpha x} = \frac{n!}{\alpha^{n+1}} \qquad \left(\frac{1}{2}\right)! = \frac{\sqrt{\pi}}{2}$$

$$\int_{-\infty}^\infty dx \exp\left[-ikx - \frac{x^2}{2\sigma^2}\right] = \sqrt{2\pi\sigma^2} \exp\left[-\frac{\sigma^2 k^2}{2}\right] \qquad \lim_{N \rightarrow \infty} \ln N! = N \ln N - N$$

$$\langle e^{-ikx} \rangle = \sum_{n=0}^\infty \frac{(-ik)^n}{n!} \langle x^n \rangle \qquad \ln \langle e^{-ikx} \rangle = \sum_{n=1}^\infty \frac{(-ik)^n}{n!} \langle x^n \rangle_c$$

$$\cosh(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \dots \qquad \sinh(x) = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \dots$$

$$\text{Surface area of a unit sphere in } d \text{ dimensions} \qquad S_d = \frac{2\pi^{d/2}}{(d/2-1)!}$$

1. *One dimensional gas:* A thermalized gas particle is suddenly confined to a one-dimensional trap. The corresponding mixed state is described by an initial density function $\rho(q, p, t = 0) = \delta(q)f(p)$, where $f(p) = \exp(-p^2/2mk_B T)/\sqrt{2\pi mk_B T}$.

(a) Starting from Liouville's equation, derive $\rho(q, p, t)$ and sketch it in the (q, p) plane.

• Liouville's equation, describing the incompressible nature of phase space density, is

$$\frac{\partial \rho}{\partial t} = -\dot{q} \frac{\partial \rho}{\partial q} - \dot{p} \frac{\partial \rho}{\partial p} = -\frac{\partial \mathcal{H}}{\partial p} \frac{\partial \rho}{\partial q} + \frac{\partial \mathcal{H}}{\partial q} \frac{\partial \rho}{\partial p} \equiv -\{\rho, \mathcal{H}\}.$$

For the gas particle confined to a 1-dimensional trap, the Hamiltonian can be written as

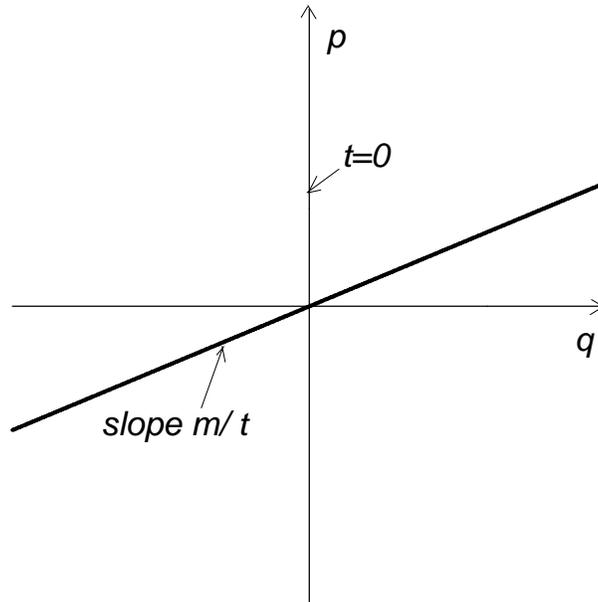
$$\mathcal{H} = \frac{p^2}{2m} + V(q_x) = \frac{p^2}{2m},$$

since $V_{q_x} = 0$, and there is no motion in the y and z directions. With this Hamiltonian, Liouville's equation becomes

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m} \frac{\partial \rho}{\partial q},$$

whose solution, subject to the specified initial conditions, is

$$\rho(q, p, t) = \rho\left(q - \frac{p}{m}t, p, 0\right) = \delta\left(q - \frac{p}{m}t\right) f(p).$$



(b) Derive the expressions for the averages $\langle q^2 \rangle$ and $\langle p^2 \rangle$ at $t > 0$.

• The expectation value for any observable \mathcal{O} is

$$\langle \mathcal{O} \rangle = \int d\Gamma \mathcal{O} \rho(\Gamma, t),$$

and hence

$$\begin{aligned}\langle p^2 \rangle &= \int p^2 f(p) \delta\left(q - \frac{p}{m}t\right) dp dq = \int p^2 f(p) dp \\ &= \int_{-\infty}^{\infty} dp p^2 \frac{1}{\sqrt{2\pi m k_B T}} \exp\left(-\frac{p^2}{2m k_B T}\right) = m k_B T.\end{aligned}$$

Likewise, we obtain

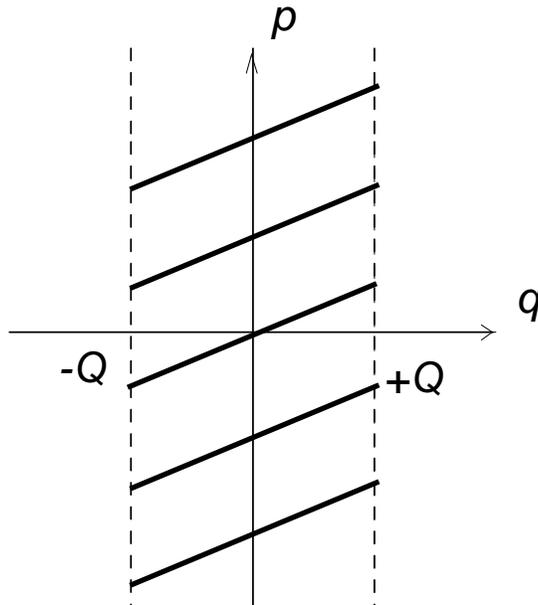
$$\langle q^2 \rangle = \int q^2 f(p) \delta\left(q - \frac{p}{m}t\right) dp dq = \int \left(\frac{p}{m}t\right)^2 f(p) dp = \left(\frac{t}{m}\right)^2 \int p^2 f(p) dp = \frac{k_B T}{m} t^2.$$

(c) Suppose that hard walls are placed at $q = \pm Q$. Describe $\rho(q, p, t \gg \tau)$, where τ is an appropriately large relaxation time.

• Now suppose that hard walls are placed at $q = \pm Q$. The appropriate relaxation time τ , is the characteristic length between the containing walls divided by the characteristic velocity of the particle, i.e.

$$\tau \sim \frac{2Q}{|\dot{q}|} = \frac{2Qm}{\sqrt{\langle p^2 \rangle}} = 2Q \sqrt{\frac{m}{k_B T}}.$$

Initially $\rho(q, p, t)$ resembles the distribution shown in part (a), but each time the particle hits the barrier, reflection changes p to $-p$. As time goes on, the slopes become less, and $\rho(q, p, t)$ becomes a set of closely spaced lines whose separation vanishes as $2mQ/t$.



(d) A “coarse-grained” density $\tilde{\rho}$, is obtained by ignoring variations of ρ below some small resolution in the (q, p) plane; e.g., by averaging ρ over cells of the resolution area. Find $\tilde{\rho}(q, p)$ for the situation in part (c), and show that it is stationary.

- We can choose any resolution ε in (p, q) space, subdividing the plane into an array of pixels of this area. For any ε , after sufficiently long time many lines will pass through this area. Averaging over them leads to

$$\tilde{\rho}(q, p, t \gg \tau) = \frac{1}{2Q} f(p),$$

as (i) the density $f(p)$ at each p is always the same, and (ii) all points along $q \in [-Q, +Q]$ are equally likely. For the time variation of this coarse-grained density, we find

$$\frac{\partial \tilde{\rho}}{\partial t} = -\frac{p}{m} \frac{\partial \tilde{\rho}}{\partial q} = 0, \quad \text{i.e. } \tilde{\rho} \text{ is stationary.}$$

2. Evolution of entropy: The normalized ensemble density is a probability in the phase space Γ . This probability has an associated entropy $S(t) = -\int d\Gamma \rho(\Gamma, t) \ln \rho(\Gamma, t)$.

(a) Show that if $\rho(\Gamma, t)$ satisfies Liouville's equation for a Hamiltonian \mathcal{H} , $dS/dt = 0$.

- A candidate “entropy” is defined by

$$S(t) = -\int d\Gamma \rho(\Gamma, t) \ln \rho(\Gamma, t) = -\langle \ln \rho(\Gamma, t) \rangle.$$

Taking the derivative with respect to time gives

$$\frac{dS}{dt} = -\int d\Gamma \left(\frac{\partial \rho}{\partial t} \ln \rho + \rho \frac{1}{\rho} \frac{\partial \rho}{\partial t} \right) = -\int d\Gamma \frac{\partial \rho}{\partial t} (\ln \rho + 1).$$

Substituting the expression for $\partial \rho / \partial t$ obtained from Liouville's theorem gives

$$\frac{dS}{dt} = -\int d\Gamma \sum_{i=1}^{3N} \left(\frac{\partial \rho}{\partial p_i} \frac{\partial \mathcal{H}}{\partial q_i} - \frac{\partial \rho}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} \right) (\ln \rho + 1).$$

(Here the index i is used to label the 3 coordinates, as well as the N particles, and hence runs from 1 to $3N$.) Integrating the above expression by parts yields[†]

[†] This is standard integration by parts, i.e. $\int_b^a F dG = FG|_b^a - \int_b^a G dF$. Looking explicitly at one term in the expression to be integrated in this problem,

$$\int \prod_{i=1}^{3N} dV_i \frac{\partial \rho}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} = \int dq_1 dp_1 \cdots dq_i dp_i \cdots dq_{3N} dp_{3N} \frac{\partial \rho}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i},$$

we identify $dG = dq_i \frac{\partial \rho}{\partial q_i}$, and F with the remainder of the expression. Noting that $\rho(q_i) = 0$ at the boundaries of the box, we get

$$\int \prod_{i=1}^{3N} dV_i \frac{\partial \rho}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} = -\int \prod_{i=1}^{3N} dV_i \rho \frac{\partial}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i}.$$

$$\begin{aligned}
\frac{dS}{dt} &= \int d\Gamma \sum_{i=1}^{3N} \left[\rho \frac{\partial}{\partial p_i} \left(\frac{\partial \mathcal{H}}{\partial q_i} (\ln \rho + 1) \right) - \rho \frac{\partial}{\partial q_i} \left(\frac{\partial \mathcal{H}}{\partial p_i} (\ln \rho + 1) \right) \right] \\
&= \int d\Gamma \sum_{i=1}^{3N} \left[\rho \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_i} (\ln \rho + 1) + \rho \frac{\partial \mathcal{H}}{\partial q_i} \frac{1}{\rho} \frac{\partial \rho}{\partial p_i} - \rho \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_i} (\ln \rho + 1) - \rho \frac{\partial \mathcal{H}}{\partial p_i} \frac{1}{\rho} \frac{\partial \rho}{\partial q_i} \right] \\
&= \int d\Gamma \sum_{i=1}^{3N} \left[\frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial \rho}{\partial p_i} - \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \rho}{\partial q_i} \right].
\end{aligned}$$

Integrating the final expression by parts gives

$$\frac{dS}{dt} = - \int d\Gamma \sum_{i=1}^{3N} \left[-\rho \frac{\partial^2 \mathcal{H}}{\partial p_i \partial q_i} + \rho \frac{\partial^2 \mathcal{H}}{\partial q_i \partial p_i} \right] = 0.$$

(b) Using the method of Lagrange multipliers, find the function $\rho_{\max}(\Gamma)$ which maximizes the functional $S[\rho]$, subject to the constraint of fixed average energy, $\langle \mathcal{H} \rangle = \int d\Gamma \rho \mathcal{H} = E$.

• There are two constraints, normalization and constant average energy, written respectively as

$$\int d\Gamma \rho(\Gamma) = 1, \quad \text{and} \quad \langle \mathcal{H} \rangle = \int d\Gamma \rho(\Gamma) \mathcal{H} = E.$$

Rewriting the expression for entropy,

$$S(t) = \int d\Gamma \rho(\Gamma) [-\ln \rho(\Gamma) - \alpha - \beta \mathcal{H}] + \alpha + \beta E,$$

where α and β are Lagrange multipliers used to enforce the two constraints. Extremizing the above expression with respect to the function $\rho(\Gamma)$, results in

$$\left. \frac{\partial S}{\partial \rho(\Gamma)} \right|_{\rho=\rho_{max}} = -\ln \rho_{max}(\Gamma) - \alpha - \beta \mathcal{H}(\Gamma) - 1 = 0.$$

The solution to this equation is

$$\ln \rho_{max} = -(\alpha + 1) - \beta \mathcal{H},$$

which can be rewritten as

$$\rho_{max} = C \exp(-\beta \mathcal{H}), \quad \text{where} \quad C = e^{-(\alpha+1)}.$$

(c) Show that the solution to part (b) is stationary, i.e. $\partial\rho_{\max}/\partial t = 0$.

• The density obtained in part (b) is stationary, as can be easily checked from

$$\begin{aligned}\frac{\partial\rho_{\max}}{\partial t} &= -\{\rho_{\max}, \mathcal{H}\} = -\{Ce^{-\beta\mathcal{H}}, \mathcal{H}\} \\ &= \frac{\partial\mathcal{H}}{\partial p}C(-\beta)\frac{\partial\mathcal{H}}{\partial q}e^{-\beta\mathcal{H}} - \frac{\partial\mathcal{H}}{\partial q}C(-\beta)\frac{\partial\mathcal{H}}{\partial p}e^{-\beta\mathcal{H}} = 0.\end{aligned}$$

(d) How can one reconcile the result in (a), with the observed increase in entropy as the system approaches the equilibrium density in (b)? (Hint: Think of the situation encountered in the previous problem.)

• Liouville's equation preserves the information content of the PDF $\rho(\Gamma, t)$, and hence $S(t)$ does not increase in time. However, as illustrated in the example in problem 1, the density becomes more finely dispersed in phase space. In the presence of any coarse-graining of phase space, information disappears. The maximum entropy, corresponding to $\tilde{\rho}$, describes equilibrium in this sense.

3. *The Vlasov equation* is obtained in the limit of high particle density $n = N/V$, or large inter-particle interaction range λ , such that $n\lambda^3 \gg 1$. In this limit, the collision terms are dropped from the left hand side of the equations in the BBGKY hierarchy.

The BBGKY hierarchy

$$\begin{aligned}\left[\frac{\partial}{\partial t} + \sum_{n=1}^s \frac{\vec{p}_n}{m} \cdot \frac{\partial}{\partial \vec{q}_n} - \sum_{n=1}^s \left(\frac{\partial U}{\partial \vec{q}_n} + \sum_l \frac{\partial \mathcal{V}(\vec{q}_n - \vec{q}_l)}{\partial \vec{q}_n} \right) \cdot \frac{\partial}{\partial \vec{p}_n} \right] f_s \\ = \sum_{n=1}^s \int dV_{s+1} \frac{\partial \mathcal{V}(\vec{q}_n - \vec{q}_{s+1})}{\partial \vec{q}_n} \cdot \frac{\partial f_{s+1}}{\partial \vec{p}_n},\end{aligned}$$

has the characteristic time scales

$$\begin{cases} \frac{1}{\tau_U} \sim \frac{\partial U}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \sim \frac{v}{L}, \\ \frac{1}{\tau_c} \sim \frac{\partial \mathcal{V}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \sim \frac{v}{\lambda}, \\ \frac{1}{\tau_X} \sim \int dx \frac{\partial \mathcal{V}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \frac{f_{s+1}}{f_s} \sim \frac{1}{\tau_c} \cdot n\lambda^3, \end{cases}$$

where $n\lambda^3$ is the number of particles within the interaction range λ , and v is a typical velocity. The Boltzmann equation is obtained in the dilute limit, $n\lambda^3 \ll 1$, by disregarding terms of order $1/\tau_X \ll 1/\tau_c$. The Vlasov equation is obtained in the dense limit of $n\lambda^3 \gg 1$ by ignoring terms of order $1/\tau_c \ll 1/\tau_X$.

(a) Assume that the N body density is a product of one particle densities, i.e. $\rho = \prod_{i=1}^N \rho_1(\mathbf{x}_i, t)$, where $\mathbf{x}_i \equiv (\vec{p}_i, \vec{q}_i)$. Calculate the densities f_s , and their normalizations.

• Let bfx_i denote the coordinates and momenta for particle i . Starting from the joint probability $\rho_N = \prod_{i=1}^N \rho_1(\mathbf{x}_i, t)$, for *independent particles*, we find

$$f_s = \frac{N!}{(N-s)!} \int \prod_{\alpha=s+1}^N dV_\alpha \rho_N = \frac{N!}{(N-s)!} \prod_{n=1}^s \rho_1(\mathbf{x}_n, t).$$

The normalizations follow from

$$\int d\Gamma \rho = 1, \quad \implies \quad \int dV_1 \rho_1(\mathbf{x}, t) = 1,$$

and

$$\int \prod_{n=1}^s dV_n f_s = \frac{N!}{(N-s)!} \approx N^s \quad \text{for} \quad s \ll N.$$

(b) Show that once the collision terms are eliminated, all the equations in the BBGKY hierarchy are equivalent to the single equation

$$\left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial}{\partial \vec{q}} - \frac{\partial U_{\text{eff}}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \right] f_1(\vec{p}, \vec{q}, t) = 0,$$

where

$$U_{\text{eff}}(\vec{q}, t) = U(\vec{q}) + \int d\mathbf{x}' \mathcal{V}(\vec{q} - \vec{q}') f_1(\mathbf{x}', t).$$

• Noting that

$$\frac{f_{s+1}}{f_s} = \frac{(N-s)!}{(N-s-1)!} \rho_1(\mathbf{x}_{s+1}),$$

the reduced BBGKY hierarchy is

$$\begin{aligned} & \left[\frac{\partial}{\partial t} + \sum_{n=1}^s \left(\frac{\vec{p}_n}{m} \cdot \frac{\partial}{\partial \vec{q}_n} - \frac{\partial U}{\partial \vec{q}_n} \cdot \frac{\partial}{\partial \vec{p}_n} \right) \right] f_s \\ & \approx \sum_{n=1}^s \int dV_{s+1} \frac{\partial \mathcal{V}(\vec{q}_n - \vec{q}_{s+1})}{\partial \vec{q}_n} \cdot \frac{\partial}{\partial \vec{p}_n} [(N-s) f_s \rho_1(\mathbf{x}_{s+1})] \\ & \approx \sum_{n=1}^s \frac{\partial}{\partial \vec{q}_n} \left[\int dV_{s+1} \rho_1(\mathbf{x}_{s+1}) \mathcal{V}(\vec{q}_n - \vec{q}_{s+1}) \cdot N \right] \frac{\partial}{\partial \vec{p}_n} f_s, \end{aligned}$$

where we have used the approximation $(N-s) \approx N$ for $N \gg s$. Rewriting the above expression,

$$\left[\frac{\partial}{\partial t} + \sum_{n=1}^s \left(\frac{\vec{p}_n}{m} \cdot \frac{\partial}{\partial \vec{q}_n} - \frac{\partial U_{\text{eff}}}{\partial \vec{q}_n} \cdot \frac{\partial}{\partial \vec{p}_n} \right) \right] f_s = 0,$$

where

$$U_{eff} = U(\vec{q}) + N \int dV' \mathcal{V}(\vec{q} - \vec{q}') \rho_1(\mathbf{x}', t).$$

(c) Now consider N particles confined to a box of volume V , with no additional potential. Show that $f_1(\vec{q}, \vec{p}) = g(\vec{p})/V$ is a stationary solution to the Vlasov equation for any $g(\vec{p})$. Why is there no relaxation towards equilibrium for $g(\vec{p})$?

- Starting from

$$\rho_1 = g(\vec{p})/V,$$

we obtain

$$\mathcal{H}_{eff} = \sum_{i=1}^N \left[\frac{\vec{p}_i^2}{2m} + U_{eff}(\vec{q}_i) \right],$$

with

$$U_{eff} = 0 + N \int dV' \mathcal{V}(\vec{q} - \vec{q}') \frac{1}{V} g(\vec{p}) = \frac{N}{V} \int d^3q \mathcal{V}(\vec{q}).$$

(We have taken advantage of the normalization $\int d^3p g(\vec{p}) = 1$.) Substituting into the Vlasov equation yields

$$\left(\frac{\partial}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial}{\partial \vec{q}} \right) \rho_1 = 0.$$

There is no relaxation towards equilibrium because there are no collisions which allow $g(\vec{p})$ to relax. The momentum of each particle is conserved by \mathcal{H}_{eff} ; i.e. $\{\rho_1, \mathcal{H}_{eff}\} = 0$, preventing its change.

4. Two component plasma: Consider a *neutral* mixture of N ions of charge $+e$ and mass m_+ , and N electrons of charge $-e$ and mass m_- , in a volume $V = N/n_0$.

(a) Show that the Vlasov equations for this two component system are

$$\begin{cases} \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m_+} \cdot \frac{\partial}{\partial \vec{q}} + e \frac{\partial \Phi_{eff}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \right] f_+(\vec{p}, \vec{q}, t) = 0 \\ \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m_-} \cdot \frac{\partial}{\partial \vec{q}} - e \frac{\partial \Phi_{eff}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \right] f_-(\vec{p}, \vec{q}, t) = 0 \end{cases},$$

where the effective Coulomb potential is given by

$$\Phi_{eff}(\vec{q}, t) = \Phi_{ext}(\vec{q}) + e \int d\mathbf{x}' C(\vec{q} - \vec{q}') [f_+(\mathbf{x}', t) - f_-(\mathbf{x}', t)].$$

Here, Φ_{ext} is the potential set up by the external charges, and the Coulomb potential $C(\vec{q})$ satisfies the differential equation $\nabla^2 C = 4\pi\delta^3(\vec{q})$.

- The Hamiltonian for the two component mixture is

$$\mathcal{H} = \sum_{i=1}^N \left[\frac{\vec{p}_i^2}{2m_+} + \frac{\vec{p}_i^2}{2m_-} \right] + \sum_{i,j=1}^{2N} e_i e_j \frac{1}{|\vec{q}_i - \vec{q}_j|} + \sum_{i=1}^{2N} e_i \Phi_{ext}(\vec{q}_i),$$

where $C(\vec{q}_i - \vec{q}_j) = 1/|\vec{q}_i - \vec{q}_j|$, resulting in

$$\frac{\partial \mathcal{H}}{\partial \vec{q}_i} = e_i \frac{\partial \Phi_{ext}}{\partial \vec{q}_i} + e_i \sum_{j \neq i} e_j \frac{\partial}{\partial \vec{q}_i} C(\vec{q}_i - \vec{q}_j).$$

Substituting this into the Vlasov equation, we obtain

$$\begin{cases} \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m_+} \cdot \frac{\partial}{\partial \vec{q}} + e \frac{\partial \Phi_{eff}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \right] f_+(\vec{p}, \vec{q}, t) = 0, \\ \left[\frac{\partial}{\partial t} + \frac{\vec{p}}{m_-} \cdot \frac{\partial}{\partial \vec{q}} - e \frac{\partial \Phi_{eff}}{\partial \vec{q}} \cdot \frac{\partial}{\partial \vec{p}} \right] f_-(\vec{p}, \vec{q}, t) = 0. \end{cases}$$

(b) Assume that the one particle densities have the stationary forms $f_{\pm} = g_{\pm}(\vec{p})n_{\pm}(\vec{q})$. Show that the effective potential satisfies the equation

$$\nabla^2 \Phi_{eff} = 4\pi \rho_{ext} + 4\pi e (n_+(\vec{q}) - n_-(\vec{q})),$$

where ρ_{ext} is the external charge density.

- Setting $f_{\pm}(\vec{p}, \vec{q}) = g_{\pm}(\vec{p})n_{\pm}(\vec{q})$, and using $\int d^3p g_{\pm}(\vec{p}) = 1$, the integrals in the effective potential simplify to

$$\Phi_{eff}(\vec{q}, t) = \Phi_{ext}(\vec{q}) + e \int d^3q' C(\vec{q} - \vec{q}') [n_+(\vec{q}') - n_-(\vec{q}')].$$

Apply ∇^2 to the above equation, and use $\nabla^2 \Phi_{ext} = 4\pi \rho_{ext}$ and $\nabla^2 C(\vec{q} - \vec{q}') = 4\pi \delta^3(\vec{q} - \vec{q}')$, to obtain

$$\nabla^2 \Phi_{eff} = 4\pi \rho_{ext} + 4\pi e [n_+(\vec{q}) - n_-(\vec{q})].$$

(c) Further assuming that the densities relax to the equilibrium Boltzmann weights $n_{\pm}(\vec{q}) = n_0 \exp[\pm \beta e \Phi_{eff}(\vec{q})]$, leads to the self-consistency condition

$$\nabla^2 \Phi_{eff} = 4\pi [\rho_{ext} + n_0 e (e^{\beta e \Phi_{eff}} - e^{-\beta e \Phi_{eff}})],$$

known as the *Poisson–Boltzmann equation*. Due to its nonlinear form, it is generally not possible to solve the Poisson–Boltzmann equation. By linearizing the exponentials, one obtains the simpler *Debye equation*

$$\nabla^2 \Phi_{eff} = 4\pi \rho_{ext} + \Phi_{eff}/\lambda^2.$$

Give the expression for the *Debye screening length* λ .

- Linearizing the Boltzmann weights gives

$$n_{\pm} = n_o \exp[\mp \beta e \Phi_{eff}(\vec{q})] \approx n_o [1 \mp \beta e \Phi_{eff}],$$

resulting in

$$\nabla^2 \Phi_{eff} = 4\pi \rho_{ext} + \frac{1}{\lambda^2} \Phi_{eff},$$

with the screening length given by

$$\lambda^2 = \frac{k_B T}{8\pi n_o e^2}.$$

(d) Show that the Debye equation has the general solution

$$\Phi_{eff}(\vec{q}) = \int d^3 \vec{q}' G(\vec{q} - \vec{q}') \rho_{ext}(\vec{q}'),$$

where $G(\vec{q}) = \exp(-|\vec{q}|/\lambda)/|\vec{q}|$ is the screened Coulomb potential.

- We want to show that the Debye equation has the general solution

$$\Phi_{eff}(\vec{q}) = \int d^3 \vec{q}' G(\vec{q} - \vec{q}') \rho_{ext}(\vec{q}'),$$

where

$$G(\vec{q}) = \frac{\exp(-|q|/\lambda)}{|q|}.$$

Effectively, we want to show that $\nabla^2 G = G/\lambda^2$ for $\vec{q} \neq 0$. In spherical coordinates, $G = \exp(-r/\lambda)/r$. Evaluating ∇^2 in spherical coordinates gives

$$\begin{aligned} \nabla^2 G &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial G}{\partial r} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \left[-\frac{1}{\lambda} \frac{e^{-r/\lambda}}{r} - \frac{e^{-r/\lambda}}{r^2} \right] \\ &= \frac{1}{r^2} \left[\frac{1}{\lambda^2} r e^{-r/\lambda} - \frac{1}{\lambda} e^{-r/\lambda} + \frac{1}{\lambda} e^{-r/\lambda} \right] = \frac{1}{\lambda^2} \frac{e^{-r/\lambda}}{r} = \frac{G}{\lambda^2}. \end{aligned}$$

(e) Give the condition for the self-consistency of the Vlasov approximation, and interpret it in terms of the inter-particle spacing?

- The Vlasov equation assumes the limit $n_o \lambda^3 \gg 1$, which requires that

$$\frac{(k_B T)^{3/2}}{n_o^{1/2} e^3} \gg 1, \quad \implies \quad \frac{e^2}{k_B T} \ll n_o^{-1/3} \sim \ell,$$

where ℓ is the interparticle spacing. In terms of the interparticle spacing, the self-consistency condition is

$$\frac{e^2}{\ell} \ll k_B T,$$

i.e. the interaction energy is much less than the kinetic (thermal) energy.

(f) Show that the characteristic relaxation time ($\tau \approx \lambda/c$) is temperature independent. What property of the plasma is it related to?

- A characteristic time is obtained from

$$\tau \sim \frac{\lambda}{c} \sim \sqrt{\frac{k_B T}{n_o e^2}} \cdot \sqrt{\frac{m}{k_B T}} \sim \sqrt{\frac{m}{n_o e^2}} \sim \frac{1}{\omega_p},$$

where ω_p is the plasma frequency.

5. Two dimensional electron gas in a magnetic field: When donor atoms (such as P or As) are added to a semiconductor (e.g. Si or Ge), their conduction electrons can be thermally excited to move freely in the host lattice. By growing layers of different materials, it is possible to generate a spatially varying potential (work-function) which traps electrons at the boundaries between layers. In the following, we shall treat the trapped electrons as a gas of classical particles *in two dimensions*.

If the layer of electrons is sufficiently separated from the donors, the main source of scattering is from electron-electron collisions.

(a) The Hamiltonian for non-interacting free electrons in a magnetic field has the form

$$\mathcal{H} = \sum_i \left[\frac{(\vec{p}_i - e\vec{A})^2}{2m} \pm \mu_B |\vec{B}| \right].$$

(The two signs correspond to electron spins parallel or anti-parallel to the field.) The vector potential $\vec{A} = \vec{B} \times \vec{q}/2$ describes a uniform magnetic field \vec{B} . Obtain the classical equations of motion, and show that they describe rotation of electrons in cyclotron orbits in a plane orthogonal to \vec{B} .

- The Hamiltonian for non-interacting free electrons in a magnetic field has the form

$$\mathcal{H} = \sum_i \left[\frac{(\vec{p}_i + e\vec{A})^2}{2m} \pm \mu_B |\vec{B}| \right],$$

or in expanded form

$$\mathcal{H} = \frac{p^2}{2m} + \frac{e}{m} \vec{p} \cdot \vec{A} + \frac{e^2}{2m} \vec{A}^2 \pm \mu_B |\vec{B}|.$$

Substituting $\vec{A} = \vec{B} \times \vec{q}/2$, results in

$$\begin{aligned}\mathcal{H} &= \frac{p^2}{2m} + \frac{e}{2m} \vec{p} \cdot \vec{B} \times \vec{q} + \frac{e^2}{8m} (\vec{B} \times \vec{q})^2 \pm \mu_B |\vec{B}| \\ &= \frac{p^2}{2m} + \frac{e}{2m} \vec{p} \times \vec{B} \cdot \vec{q} + \frac{e^2}{8m} (B^2 q^2 - (\vec{B} \cdot \vec{q})^2) \pm \mu_B |\vec{B}|.\end{aligned}$$

Using the canonical equations, $\dot{\vec{q}} = \partial\mathcal{H}/\partial\vec{p}$ and $\dot{\vec{p}} = -\partial\mathcal{H}/\partial\vec{q}$, we find

$$\begin{cases} \dot{\vec{q}} = \frac{\partial\mathcal{H}}{\partial\vec{p}} = \frac{\vec{p}}{m} + \frac{e}{2m} \vec{B} \times \vec{q}, & \implies \vec{p} = m\dot{\vec{q}} - \frac{e}{2} \vec{B} \times \vec{q}, \\ \dot{\vec{p}} = -\frac{\partial\mathcal{H}}{\partial\vec{q}} = -\frac{e}{2m} \vec{p} \times \vec{B} - \frac{e^2}{4m} B^2 \vec{q} + \frac{e^2}{4m} (\vec{B} \cdot \vec{q}) \vec{B}. \end{cases}$$

Differentiating the first expression obtained for \vec{p} , and setting it equal to the second expression for $\dot{\vec{p}}$ above, gives

$$m\ddot{\vec{q}} - \frac{e}{2} \vec{B} \times \dot{\vec{q}} = -\frac{e}{2m} \left(m\dot{\vec{q}} - \frac{e}{2} \vec{B} \times \vec{q} \right) \times \vec{B} - \frac{e^2}{4m} |\vec{B}|^2 \vec{q} + \frac{e^2}{4m} (\vec{B} \cdot \vec{q}) \vec{B}.$$

Simplifying the above expression, using $\vec{B} \times \vec{q} \times \vec{B} = B^2 \vec{q} - (\vec{B} \cdot \vec{q}) \vec{B}$, leads to

$$m\ddot{\vec{q}} = e\vec{B} \times \dot{\vec{q}}.$$

This describes the rotation of electrons in cyclotron orbits,

$$\ddot{\vec{q}} = \vec{\omega}_c \times \dot{\vec{q}},$$

where $\vec{\omega}_c = e\vec{B}/m$; i.e. rotations are in the plane perpendicular to \vec{B} .

(b) Write down heuristically (i.e. not through a step by step derivation), the Boltzmann equations for the densities $f_{\uparrow}(\vec{p}, \vec{q}, t)$ and $f_{\downarrow}(\vec{p}, \vec{q}, t)$ of electrons with up and down spins, in terms of the two cross-sections $\sigma \equiv \sigma_{\uparrow\uparrow} = \sigma_{\downarrow\downarrow}$, and $\sigma_{\times} \equiv \sigma_{\uparrow\downarrow}$, of *spin conserving* collisions.

• Consider the classes of collisions described by cross-sections $\sigma \equiv \sigma_{\uparrow\uparrow} = \sigma_{\downarrow\downarrow}$, and $\sigma_{\times} \equiv \sigma_{\uparrow\downarrow}$. We can write the Boltzmann equations for the densities as

$$\begin{aligned}\frac{\partial f_{\uparrow}}{\partial t} - \{\mathcal{H}_{\uparrow}, f_{\uparrow}\} &= \int d^2 p_2 d\Omega |v_1 - v_2| \left\{ \frac{d\sigma}{d\Omega} [f_{\uparrow}(\vec{p}_1') f_{\uparrow}(\vec{p}_2') - f_{\uparrow}(\vec{p}_1) f_{\uparrow}(\vec{p}_2)] + \right. \\ &\quad \left. \frac{d\sigma_{\times}}{d\Omega} [f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2') - f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2)] \right\},\end{aligned}$$

and

$$\frac{\partial f_{\downarrow}}{\partial t} - \{\mathcal{H}_{\downarrow}, f_{\downarrow}\} = \int d^2 p_2 d\Omega |v_1 - v_2| \left\{ \frac{d\sigma}{d\Omega} [f_{\downarrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2') - f_{\downarrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2)] + \right.$$

$$\frac{d\sigma_{\times}}{d\Omega} [f_{\downarrow}(\vec{p}_1') f_{\uparrow}(\vec{p}_2') - f_{\downarrow}(\vec{p}_1) f_{\uparrow}(\vec{p}_2)] \Big\}.$$

(c) Show that $dH/dt \leq 0$, where $H = H_{\uparrow} + H_{\downarrow}$ is the sum of the corresponding H functions.

- The usual Boltzmann H–Theorem states that $dH/dt \leq 0$, where

$$H = \int d^2q d^2p f(\vec{q}, \vec{p}, t) \ln f(\vec{q}, \vec{p}, t).$$

For the electron gas in a magnetic field, the H function can be generalized to

$$H = \int d^2q d^2p [f_{\uparrow} \ln f_{\uparrow} + f_{\downarrow} \ln f_{\downarrow}],$$

where the condition $dH/dt \leq 0$ is proved as follows:

$$\begin{aligned} \frac{dH}{dt} &= \int d^2q d^2p \left[\frac{\partial f_{\uparrow}}{\partial t} (\ln f_{\uparrow} + 1) + \frac{\partial f_{\downarrow}}{\partial t} (\ln f_{\downarrow} + 1) \right] \\ &= \int d^2q d^2p [(\ln f_{\uparrow} + 1) (\{f_{\uparrow}, \mathcal{H}_{\uparrow}\} + C_{\uparrow\uparrow} + C_{\uparrow\downarrow}) + (\ln f_{\downarrow} + 1) (\{f_{\downarrow}, \mathcal{H}_{\downarrow}\} + C_{\downarrow\downarrow} + C_{\downarrow\uparrow})], \end{aligned}$$

with $C_{\uparrow\uparrow}$, etc., defined via the right hand side of the equations in part (b). Hence

$$\begin{aligned} \frac{dH}{dt} &= \int d^2q d^2p (\ln f_{\uparrow} + 1) (C_{\uparrow\uparrow} + C_{\uparrow\downarrow}) + (\ln f_{\downarrow} + 1) (C_{\downarrow\downarrow} + C_{\downarrow\uparrow}) \\ &= \int d^2q d^2p (\ln f_{\uparrow} + 1) C_{\uparrow\uparrow} + (\ln f_{\downarrow} + 1) C_{\downarrow\downarrow} + (\ln f_{\uparrow} + 1) C_{\uparrow\downarrow} + (\ln f_{\downarrow} + 1) C_{\downarrow\uparrow} \\ &\equiv \frac{dH_{\uparrow\uparrow}}{dt} + \frac{dH_{\downarrow\downarrow}}{dt} + \frac{d}{dt} (H_{\uparrow\downarrow} + H_{\downarrow\uparrow}), \end{aligned}$$

where the H's are in correspondence to the integrals for the collisions. We have also made use of the fact that $\int d^2p d^2q \{f_{\uparrow}, \mathcal{H}_{\uparrow}\} = \int d^2p d^2q \{f_{\downarrow}, \mathcal{H}_{\downarrow}\} = 0$. Dealing with each of the terms in the final equation individually,

$$\frac{dH_{\uparrow\uparrow}}{dt} = \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| (\ln f_{\uparrow} + 1) \frac{d\sigma}{d\Omega} [f_{\uparrow}(\vec{p}_1') f_{\uparrow}(\vec{p}_2') - f_{\uparrow}(\vec{p}_1) f_{\uparrow}(\vec{p}_2)].$$

After symmetrizing this equation, as done in the text,

$$\begin{aligned} \frac{dH_{\uparrow\uparrow}}{dt} &= -\frac{1}{4} \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| \frac{d\sigma}{d\Omega} [\ln f_{\uparrow}(\vec{p}_1) f_{\uparrow}(\vec{p}_2) - \ln f_{\uparrow}(\vec{p}_1') f_{\uparrow}(\vec{p}_2')] \\ &\quad \cdot [f_{\uparrow}(\vec{p}_1) f_{\uparrow}(\vec{p}_2) - f_{\uparrow}(\vec{p}_1') f_{\uparrow}(\vec{p}_2')] \leq 0. \end{aligned}$$

Similarly, $dH_{\downarrow\downarrow}/dt \leq 0$. Dealing with the two remaining terms,

$$\begin{aligned}\frac{dH_{\uparrow\downarrow}}{dt} &= \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| [\ln f_{\uparrow}(\vec{p}_1) + 1] \frac{d\sigma_{\times}}{d\Omega} [f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2') - f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2)] \\ &= \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| [\ln f_{\uparrow}(\vec{p}_1') + 1] \frac{d\sigma_{\times}}{d\Omega} [f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2) - f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2')],\end{aligned}$$

where we have exchanged $(\vec{p}_1, \vec{p}_2 \leftrightarrow \vec{p}_1', \vec{p}_2')$. Averaging these two expressions together,

$$\begin{aligned}\frac{dH_{\uparrow\downarrow}}{dt} &= -\frac{1}{2} \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| \frac{d\sigma_{\times}}{d\Omega} [\ln f_{\uparrow}(\vec{p}_1) - \ln f_{\uparrow}(\vec{p}_1')] \\ &\quad \cdot [f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2) - f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2')].\end{aligned}$$

Likewise

$$\begin{aligned}\frac{dH_{\downarrow\uparrow}}{dt} &= -\frac{1}{2} \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| \frac{d\sigma_{\times}}{d\Omega} [\ln f_{\downarrow}(\vec{p}_2) - \ln f_{\downarrow}(\vec{p}_2')] \\ &\quad \cdot [f_{\downarrow}(\vec{p}_2) f_{\uparrow}(\vec{p}_1) - f_{\downarrow}(\vec{p}_2') f_{\uparrow}(\vec{p}_1')].\end{aligned}$$

Combining these two expressions,

$$\begin{aligned}\frac{d}{dt} (H_{\uparrow\downarrow} + H_{\downarrow\uparrow}) &= -\frac{1}{4} \int d^2q d^2p_1 d^2p_2 d\Omega |v_1 - v_2| \frac{d\sigma_{\times}}{d\Omega} \\ &\quad [\ln f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2) - \ln f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2')] [f_{\uparrow}(\vec{p}_1) f_{\downarrow}(\vec{p}_2) - f_{\uparrow}(\vec{p}_1') f_{\downarrow}(\vec{p}_2')] \leq 0.\end{aligned}$$

Since each contribution is separately negative, we have

$$\frac{dH}{dt} = \frac{dH_{\uparrow\uparrow}}{dt} + \frac{dH_{\downarrow\downarrow}}{dt} + \frac{d}{dt} (H_{\uparrow\downarrow} + H_{\downarrow\uparrow}) \leq 0.$$

(d) Show that $dH/dt = 0$ for any $\ln f$ which is, *at each location*, a linear combination of quantities conserved in the collisions.

- For $dH/dt = 0$ we need each of the three square brackets in the previous derivation to be zero. The first two contributions, from $dH_{\uparrow\downarrow}/dt$ and $dH_{\downarrow\uparrow}/dt$, are similar to those discussed in the notes for a single particle, and vanish for any $\ln f$ which is a linear combination of quantities conserved in collisions

$$\ln f_{\alpha} = \sum_i a_i^{\alpha}(\vec{q}) \chi_i(\vec{p}),$$

where $\alpha = (\uparrow \text{ or } \downarrow)$. Clearly at each location \vec{q} , for such f_{α} ,

$$\ln f_{\alpha}(\vec{p}_1) + \ln f_{\alpha}(\vec{p}_2) = \ln f_{\alpha}(\vec{p}_1') + \ln f_{\alpha}(\vec{p}_2').$$

If we consider only the first two terms of $dH/dt = 0$, the coefficients $a_i^\alpha(\vec{q})$ can vary with both \vec{q} and $\alpha = (\uparrow \text{ or } \downarrow)$. This changes when we consider the third term $d(H_{\uparrow\downarrow} + H_{\downarrow\uparrow})/dt$. The conservations of momentum and kinetic energy constrain the corresponding four functions to be the same, i.e. they require $a_i^\uparrow(\vec{q}) = a_i^\downarrow(\vec{q})$. There is, however, no similar constraint for the overall constant that comes from particle number conservation, as the numbers of spin-up and spin-down particles is *separately* conserved, i.e. $a_0^\uparrow(\vec{q}) = a_0^\downarrow(\vec{q})$. This implies that the densities of up and down spins can be different in the final equilibrium, while the two systems must share the same velocity and temperature.

(e) Show that the streaming terms in the Boltzmann equation are zero for any function that depends only on the quantities conserved by the one body Hamiltonians.

- The Boltzmann equation is

$$\frac{\partial f_\alpha}{\partial t} = -\{f_\alpha, \mathcal{H}_\alpha\} + C_{\alpha\alpha} + C_{\alpha\beta},$$

where the right hand side consists of streaming terms $\{f_\alpha, \mathcal{H}_\alpha\}$, and collision terms C . Let I_i denote any quantity conserved by the one body Hamiltonian, i.e. $\{I_i, \mathcal{H}_\alpha\} = 0$. Consider f_α which is a function only of the I_i 's

$$f_\alpha \equiv f_\alpha(I_1, I_2, \dots).$$

Then

$$\{f_\alpha, \mathcal{H}_\alpha\} = \sum_j \frac{\partial f_\alpha}{\partial I_j} \{I_j, \mathcal{H}_\alpha\} = 0.$$

(f) Show that angular momentum $\vec{L} = \vec{q} \times \vec{p}$, is conserved during, and away from collisions.

- Conservation of momentum for a collision at \vec{q}

$$(\vec{p}_1 + \vec{p}_2) = (\vec{p}_1' + \vec{p}_2'),$$

implies

$$\vec{q} \times (\vec{p}_1 + \vec{p}_2) = \vec{q} \times (\vec{p}_1' + \vec{p}_2'),$$

or

$$\vec{L}_1 + \vec{L}_2 = \vec{L}_1' + \vec{L}_2',$$

where we have used $\vec{L}_i = \vec{q} \times \vec{p}_i$. Hence angular momentum \vec{L} is conserved during collisions. Note that only the z -component L_z is present for electrons moving in 2-dimensions, $\vec{q} \equiv (x_1, x_2)$, as is the case for the electron gas studied in this problem. Consider the Hamiltonian discussed in (a)

$$\mathcal{H} = \frac{p^2}{2m} + \frac{e}{2m} \vec{p} \times \vec{B} \cdot \vec{q} + \frac{e^2}{8m} \left(B^2 q^2 - (\vec{B} \cdot \vec{q})^2 \right) \pm \mu_B |\vec{B}|.$$

Let us evaluate the Poisson brackets of the individual terms with $L_z = \vec{q} \times \vec{p} \cdot \hat{z}$. The first term is

$$\{|\vec{p}|^2, \vec{q} \times \vec{p}\} = \varepsilon_{ijk} \{p_i p_l, x_j p_k\} = \varepsilon_{ijk} 2p_l \frac{\partial}{\partial x_l} (x_j p_k) = 2\varepsilon_{ilk} p_l p_k = 0,$$

where we have used $\varepsilon_{ijk} p_j p_k = 0$ since $p_j p_k = p_k p_j$ is symmetric. The second term is proportional to L_z ,

$$\{\vec{p} \times \vec{B} \cdot \vec{q}, L_z\} = \{B_z L_z, L_z\} = 0.$$

The final terms are proportional to q^2 , and $\{q^2, \vec{q} \times \vec{p}\} = 0$ for the same reason that $\{p^2, \vec{q} \times \vec{p}\} = 0$, leading to

$$\{\mathcal{H}, \vec{q} \times \vec{p}\} = 0.$$

Hence angular momentum is conserved away from collisions as well.

(g) Write down the most general form for the equilibrium distribution functions for particles confined to a circularly symmetric potential.

- The most general form of the equilibrium distribution functions must set both the collision terms, and the streaming terms to zero. Based on the results of the previous parts, we thus obtain

$$f_\alpha = A_\alpha \exp[-\beta \mathcal{H}_\alpha - \gamma L_z].$$

The collision terms allow for the possibility of a term $-\vec{u} \cdot \vec{p}$ in the exponent, corresponding to an average velocity. Such a term will not commute with the potential set up by a stationary box, and is thus ruled out by the streaming terms. On the other hand, the angular momentum does commute with a circular potential $\{V(\vec{q}), L\} = 0$, and is allowed by the streaming terms. A non-zero γ describes the electron gas rotating in a circular box.

(h) How is the result in part (g) modified by including scattering from magnetic and non-magnetic impurities?

- Scattering from any impurity removes the conservation of \vec{p} , and hence \vec{L} , in collisions. The γ term will no longer be needed. Scattering from magnetic impurities mixes populations of up and down spins, necessitating $A_\uparrow = A_\downarrow$; non-magnetic impurities do not have this effect.

(i) Do conservation of spin and angular momentum lead to new hydrodynamic equations?

- Conservation of angular momentum is related to conservation of \vec{p} , as shown in (f), and hence does not lead to any new equation. In contrast, conservation of spin leads to an additional hydrodynamic equation involving the magnetization, which is proportional to $(n_\uparrow - n_\downarrow)$.

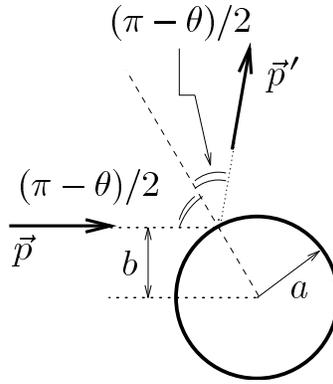
6. *The Lorentz gas* describes non-interacting particles colliding with a fixed set of scatterers. It is a good model for scattering of electrons from donor impurities. Consider a uniform two dimensional density n_0 of fixed impurities, which are hard circles of radius a .

(a) Show that the differential cross section of a hard circle scattering through an angle θ is

$$d\sigma = \frac{a}{2} \sin \frac{\theta}{2} d\theta,$$

and calculate the total cross section.

- Let b denote the impact parameter, which (see figure) is related to the angle θ between \vec{p}' and \vec{p} by



$$b(\theta) = a \sin \frac{\pi - \theta}{2} = a \cos \frac{\theta}{2}.$$

The differential cross section is then given by

$$d\sigma = 2|db| = a \sin \frac{\theta}{2} d\theta.$$

Hence the total cross section

$$\sigma_{tot} = \int_0^\pi d\theta a \sin \frac{\theta}{2} = 2a \left[-\cos \frac{\theta}{2} \right]_0^\pi = 2a.$$

(b) Write down the Boltzmann equation for the one particle density $f(\vec{q}, \vec{p}, t)$ of the Lorentz gas (including only collisions with the fixed impurities). (*Ignore the electron spin.*)

- The corresponding Boltzmann equation is

$$\begin{aligned} \frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial f}{\partial \vec{q}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} \\ = \int d\theta \frac{d\sigma}{d\theta} \frac{|\vec{p}'|}{m} n_0 [-f(\vec{p}) + f(\vec{p}')] = \frac{n_0 |\vec{p}'|}{m} \int d\theta \frac{d\sigma}{d\theta} [f(\vec{p}') - f(\vec{p})] \equiv C[f(\vec{p})]. \end{aligned}$$

(c) Using the definitions $\vec{F} \equiv -\partial U/\partial \vec{q}$, and

$$n(\vec{q}, t) = \int d^2 \vec{p} f(\vec{q}, \vec{p}, t), \quad \text{and} \quad \langle g(\vec{q}, t) \rangle = \frac{1}{n(\vec{q}, t)} \int d^2 \vec{p} f(\vec{q}, \vec{p}, t) g(\vec{q}, t),$$

show that for any function $\chi(|\vec{p}|)$, we have

$$\frac{\partial}{\partial t} (n \langle \chi \rangle) + \frac{\partial}{\partial \vec{q}} \cdot \left(n \left\langle \frac{\vec{p}}{m} \chi \right\rangle \right) = \vec{F} \cdot \left(n \left\langle \frac{\partial \chi}{\partial \vec{p}} \right\rangle \right).$$

• Using the definitions $\vec{F} \equiv -\partial U/\partial \vec{q}$,

$$n(\vec{q}, t) = \int d^2 \vec{p} f(\vec{q}, \vec{p}, t), \quad \text{and} \quad \langle g(\vec{q}, t) \rangle = \frac{1}{n(\vec{q}, t)} \int d^2 \vec{p} f(\vec{q}, \vec{p}, t) g(\vec{q}, t),$$

we can write

$$\begin{aligned} \frac{d}{dt} (n \langle \chi(|\vec{p}|) \rangle) &= \int d^2 p \chi(|\vec{p}|) \left[-\frac{\vec{p}}{m} \cdot \frac{\partial f}{\partial \vec{q}} - \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} + \int d\theta \frac{d\sigma}{d\theta} \frac{|\vec{p}|}{m} n_o (f(\vec{p}) - f(\vec{p}')) \right] \\ &= -\frac{\partial}{\partial \vec{q}} \cdot \left(n \left\langle \frac{\vec{p}}{m} \chi \right\rangle \right) + \vec{F} \cdot \left(n \left\langle \frac{\partial \chi}{\partial \vec{p}} \right\rangle \right). \end{aligned}$$

Rewriting this final expression gives the hydrodynamic equation

$$\frac{\partial}{\partial t} (n \langle \chi \rangle) + \frac{\partial}{\partial \vec{q}} \cdot \left(n \left\langle \frac{\vec{p}}{m} \chi \right\rangle \right) = \vec{F} \cdot \left(n \left\langle \frac{\partial \chi}{\partial \vec{p}} \right\rangle \right).$$

(d) Derive the conservation equation for local density $\rho \equiv mn(\vec{q}, t)$, in terms of the local velocity $\vec{u} \equiv \langle \vec{p}/m \rangle$.

• Using $\chi = 1$ in the above expression

$$\frac{\partial}{\partial t} n + \frac{\partial}{\partial \vec{q}} \cdot \left(n \left\langle \frac{\vec{p}}{m} \right\rangle \right) = 0.$$

In terms of the local density $\rho = mn$, and velocity $\vec{u} \equiv \langle \vec{p}/m \rangle$, we have

$$\frac{\partial}{\partial t} \rho + \frac{\partial}{\partial \vec{q}} \cdot (\rho \vec{u}) = 0.$$

(e) Since the magnitude of particle momentum is unchanged by impurity scattering, the Lorentz gas has an infinity of conserved quantities $|\vec{p}|^m$. This unrealistic feature is removed

upon inclusion of particle–particle collisions. For the rest of this problem focus only on $p^2/2m$ as a conserved quantity. Derive the conservation equation for the energy density

$$\epsilon(\vec{q}, t) \equiv \frac{\rho}{2} \langle c^2 \rangle, \quad \text{where} \quad \vec{c} \equiv \frac{\vec{p}}{m} - \vec{u},$$

in terms of the energy flux $\vec{h} \equiv \rho \langle \vec{c} c^2 \rangle / 2$, and the pressure tensor $P_{\alpha\beta} \equiv \rho \langle c_\alpha c_\beta \rangle$.

• With the kinetic energy $\chi = p^2/2m$ as a conserved quantity, the equation found in (c) gives

$$\frac{\partial}{\partial t} \left(\frac{n}{2m} \langle |\vec{p}|^2 \rangle \right) + \frac{\partial}{\partial \vec{q}} \cdot \left(\frac{n}{2} \left\langle \frac{\vec{p}}{m} \frac{p^2}{m} \right\rangle \right) = \vec{F} \cdot \left(n \frac{\langle \vec{p} \rangle}{m} \right).$$

Substituting $\vec{p}/m = \vec{u} + \vec{c}$, where $\langle \vec{c} \rangle = 0$, and using $\rho = nm$,

$$\frac{\partial}{\partial t} \left[\frac{\rho}{2} u^2 + \frac{\rho}{2} \langle c^2 \rangle \right] + \frac{\partial}{\partial \vec{q}} \cdot \left[\frac{\rho}{2} \langle (\vec{u} + \vec{c})(u^2 + c^2 + 2\vec{u} \cdot \vec{c}) \rangle \right] = \frac{\rho}{m} \vec{F} \cdot \vec{u}.$$

From the definition $\epsilon = \rho \langle c^2 \rangle / 2$, we have

$$\frac{\partial}{\partial t} \left[\frac{\rho}{2} u^2 + \epsilon \right] + \frac{\partial}{\partial \vec{q}} \cdot \left[\frac{\rho}{2} (\vec{u} u^2 + \vec{u} \langle c^2 \rangle + \langle \vec{c} c^2 \rangle + 2\vec{u} \cdot \langle \vec{c} \vec{c} \rangle) \right] = \frac{\rho}{m} \vec{F} \cdot \vec{u}.$$

Finally, by substituting $\vec{h} \equiv \rho \langle \vec{c} c^2 \rangle / 2$ and $P_{\alpha\beta} = \rho \langle c_\alpha c_\beta \rangle$, we get

$$\frac{\partial}{\partial t} \left[\frac{\rho}{2} u^2 + \epsilon \right] + \frac{\partial}{\partial \vec{q}} \cdot \left[\vec{u} \left(\frac{\rho}{2} u^2 + \epsilon \right) + \vec{h} \right] + \frac{\partial}{\partial q_\alpha} (u_\beta P_{\alpha\beta}) = \frac{\rho}{m} \vec{F} \cdot \vec{u}.$$

(f) Starting with a one particle density

$$f^0(\vec{p}, \vec{q}, t) = n(\vec{q}, t) \exp \left[-\frac{p^2}{2mk_B T(\vec{q}, t)} \right] \frac{1}{2\pi mk_B T(\vec{q}, t)},$$

reflecting local equilibrium conditions, calculate \vec{u} , \vec{h} , and $P_{\alpha\beta}$. Hence obtain the zeroth order hydrodynamic equations.

• There are only two quantities, 1 and $p^2/2m$, conserved in collisions. Let us start with the one particle density

$$f^0(\vec{p}, \vec{q}, t) = n(\vec{q}, t) \exp \left[-\frac{p^2}{2mk_B T(\vec{q}, t)} \right] \frac{1}{2\pi mk_B T(\vec{q}, t)}.$$

Then

$$\vec{u} = \left\langle \frac{\vec{p}}{m} \right\rangle_0 = 0, \quad \text{and} \quad \vec{h} = \left\langle \frac{\vec{p}}{m} \frac{p^2}{m} \right\rangle_0 \frac{\rho}{2} = 0,$$

since both are odd functions of \vec{p} , while f^o is an even function of \vec{p} , while

$$P_{\alpha\beta} = \rho \langle c_\alpha c_\beta \rangle = \frac{n}{m} \langle p_\alpha p_\beta \rangle = \frac{n}{m} \delta_{\alpha\beta} \cdot mk_B T = nk_B T \delta_{\alpha\beta}.$$

Substituting these expressions into the results for (c) and (d), we obtain the zeroth-order hydrodynamic equations

$$\begin{cases} \frac{\partial \rho}{\partial t} = 0, \\ \frac{\partial}{\partial t} \varepsilon = \frac{\partial}{\partial t} \frac{\rho}{2} \langle c^2 \rangle = 0. \end{cases}$$

The above equations imply that ρ and ε are independent of time, i.e.

$$\rho = n(\vec{q}), \quad \text{and} \quad \varepsilon = k_B T(\vec{q}),$$

or

$$f^0 = \frac{n(\vec{q})}{2\pi m k_B T(\vec{q})} \exp \left[-\frac{p^2}{2m k_B T(\vec{q})} \right].$$

(g) Show that in the single collision time approximation to the collision term in the Boltzmann equation, the first order solution is

$$f^1(\vec{p}, \vec{q}, t) = f^0(\vec{p}, \vec{q}, t) \left[1 - \tau \frac{\vec{p}}{m} \cdot \left(\frac{\partial \ln \rho}{\partial \vec{q}} - \frac{\partial \ln T}{\partial \vec{q}} + \frac{p^2}{2m k_B T^2} \frac{\partial T}{\partial \vec{q}} - \frac{\vec{F}}{k_B T} \right) \right].$$

• The single collision time approximation is

$$C[f] = \frac{f^0 - f}{\tau}.$$

The first order solution to Boltzmann equation

$$f = f^0 (1 + g),$$

is obtained from

$$\mathcal{L}[f^0] = -\frac{f^0 g}{\tau},$$

as

$$g = -\tau \frac{1}{f^0} \mathcal{L}[f^0] = -\tau \left[\frac{\partial}{\partial t} \ln f^0 + \frac{\vec{p}}{m} \cdot \frac{\partial}{\partial \vec{q}} \ln f^0 + \vec{F} \cdot \frac{\partial}{\partial \vec{p}} \ln f^0 \right].$$

Noting that

$$\ln f^0 = -\frac{p^2}{2m k_B T} + \ln n - \ln T - \ln(2\pi m k_B),$$

where n and T are independent of t , we have $\partial \ln f^0 / \partial t = 0$, and

$$\begin{aligned} g &= -\tau \left\{ \vec{F} \cdot \left(\frac{-\vec{p}}{mk_B T} \right) + \frac{\vec{p}}{m} \cdot \left[\frac{1}{n} \frac{\partial n}{\partial \vec{q}} - \frac{1}{T} \frac{\partial T}{\partial \vec{q}} + \frac{p^2}{2mk_B T^2} \frac{\partial T}{\partial \vec{q}} \right] \right\} \\ &= -\tau \left\{ \frac{\vec{p}}{m} \cdot \left(\frac{1}{\rho} \frac{\partial \rho}{\partial \vec{q}} - \frac{1}{T} \frac{\partial T}{\partial \vec{q}} + \frac{p^2}{2mk_B T^2} \frac{\partial T}{\partial \vec{q}} - \frac{\vec{F}}{k_B T} \right) \right\}. \end{aligned}$$

(h) Show that using the first order expression for f , we obtain

$$\rho \vec{u} = n\tau \left[\vec{F} - k_B T \nabla \ln(\rho T) \right].$$

• Clearly $\int d^2 q f^0 (1 + g) = \int d^2 q f^0 = n$, and

$$\begin{aligned} u_\alpha &= \left\langle \frac{p_\alpha}{m} \right\rangle = \frac{1}{n} \int d^2 p \frac{p_\alpha}{m} f^0 (1 + g) \\ &= \frac{1}{n} \int d^2 p \frac{p_\alpha}{m} \left[-\tau \frac{p_\beta}{m} \left(\frac{\partial \ln \rho}{\partial q_\beta} - \frac{\partial \ln T}{\partial q_\beta} - \frac{F_\beta}{k_B T} + \frac{p^2}{2mk_B T^2} \frac{\partial T}{\partial q_\beta} \right) \right] f^0. \end{aligned}$$

Wick's theorem can be used to check that

$$\begin{aligned} \langle p_\alpha p_\beta \rangle_0 &= \delta_{\alpha\beta} m k_B T, \\ \langle p^2 p_\alpha p_\beta \rangle_0 &= (m k_B T)^2 [2\delta_{\alpha\beta} + 2\delta_{\alpha\beta}] = 4\delta_{\alpha\beta} (m k_B T)^2, \end{aligned}$$

resulting in

$$u_\alpha = -\frac{n\tau}{\rho} \left[\delta_{\alpha\beta} k_B T \left(\frac{\partial}{\partial q_\beta} \ln \left(\frac{\rho}{T} \right) - \frac{1}{k_B T} F_\beta \right) + 2k_B \frac{\partial T}{\partial q_\beta} \delta_{\alpha\beta} \right].$$

Rearranging these terms yields

$$\rho u_\alpha = n\tau \left[F_\alpha - k_B T \frac{\partial}{\partial q_\alpha} \ln(\rho T) \right].$$

(i) From the above equation, calculate the velocity response function $\chi_{\alpha\beta} = \partial u_\alpha / \partial F_\beta$.

• The velocity response function is now calculated easily as

$$\chi_{\alpha\beta} = \frac{\partial u_\alpha}{\partial F_\beta} = \frac{n\tau}{\rho} \delta_{\alpha\beta}.$$

(j) Calculate $P_{\alpha\beta}$, and \vec{h} , and hence write down the first order hydrodynamic equations.

- The first order expressions for pressure tensor and heat flux are

$$P_{\alpha\beta} = \frac{\rho}{m^2} \langle p_\alpha p_\beta \rangle = \delta_{\alpha\beta} n k_B T, \quad \text{and} \quad \delta^1 P_{\alpha\beta} = 0,$$

$$h_\alpha = \frac{\rho}{2m^3} \langle p_\alpha p^2 \rangle = -\frac{\tau\rho}{2m^3} \left\langle p_\alpha p^2 \frac{p_i}{m} (a_i + b_i p^2) \right\rangle_0.$$

The latter is calculated from Wick's theorem results

$$\langle p_i p_\alpha p^2 \rangle = 4\delta_{\alpha i} (m k_B T)^2, \quad \text{and}$$

$$\langle p_i p_\alpha p^2 p^2 \rangle = (m k_B T)^3 [\delta_{\alpha i} (4 + 2) + 4 \times 2\delta_{\alpha i} + 4 \times 2\delta_{\alpha i}] = 22\delta_{\alpha i},$$

as

$$h_\alpha = -\frac{\rho\tau}{2m^3} \left[(m k_B T)^2 \left(\frac{\partial}{\partial q_\alpha} \ln \frac{\rho}{T} - \vec{F} \right) + \frac{22(m k_B T)^3}{2m k_B T} \frac{\partial}{\partial q_\alpha} \ln T \right]$$

$$= -11n k_B^2 T \tau \frac{\partial T}{\partial q_\alpha}.$$

Substitute these expressions for $P_{\alpha\beta}$ and h_α into the equation obtained in (e)

$$\frac{\partial}{\partial t} \left[\frac{\rho}{2} u^2 + \epsilon \right] + \frac{\partial}{\partial \vec{q}} \cdot \left[\vec{u} \left(\frac{\rho}{2} u^2 + \epsilon \right) - 11n k_B^2 T \tau \frac{\partial T}{\partial \vec{q}} \right] + \frac{\partial}{\partial \vec{q}} (\vec{u} n k_B T) = \frac{\rho}{m} \vec{F} \cdot \vec{u}.$$

7. Thermal conductivity: Consider a classical gas between two plates separated by a distance w . One plate at $y = 0$ is maintained at a temperature T_1 , while the other plate at $y = w$ is at a different temperature T_2 . The gas velocity is zero, so that the initial zeroth order approximation to the one particle density is,

$$f_1^0(\vec{p}, x, y, z) = \frac{n(y)}{[2\pi m k_B T(y)]^{3/2}} \exp \left[-\frac{\vec{p} \cdot \vec{p}}{2m k_B T(y)} \right].$$

(a) What is the necessary relation between $n(y)$ and $T(y)$ to ensure that the gas velocity \vec{u} remains zero? (Use this relation between $n(y)$ and $T(y)$ in the remainder of this problem.)

- Since there is no external force acting on the gas between plates, the gas can only flow locally if there are variations in pressure. Since the local pressure is $P(y) = n(y)k_B T(y)$, the condition for the fluid to be stationary is

$$n(y)T(y) = \text{constant}.$$

(b) Using Wick's theorem, or otherwise, show that

$$\langle p^2 \rangle^0 \equiv \langle p_\alpha p_\alpha \rangle^0 = 3(mk_B T), \quad \text{and} \quad \langle p^4 \rangle^0 \equiv \langle p_\alpha p_\alpha p_\beta p_\beta \rangle^0 = 15(mk_B T)^2,$$

where $\langle \mathcal{O} \rangle^0$ indicates local averages with the Gaussian weight f_1^0 . Use the result $\langle p^6 \rangle^0 = 105(mk_B T)^3$ in conjunction with symmetry arguments to conclude

$$\langle p_y^2 p^4 \rangle^0 = 35(mk_B T)^3.$$

• The Gaussian weight has a covariance $\langle p_\alpha p_\beta \rangle^0 = \delta_{\alpha\beta}(mk_B T)$. Using Wick's theorem gives

$$\langle p^2 \rangle^0 = \langle p_\alpha p_\alpha \rangle^0 = (mk_B T) \delta_{\alpha\alpha} = 3(mk_B T).$$

Similarly

$$\langle p^4 \rangle^0 = \langle p_\alpha p_\alpha p_\beta p_\beta \rangle^0 = (mk_B T)^2 (\delta_{\alpha\alpha} + 2\delta_{\alpha\beta}\delta_{\alpha\beta}) = 15(mk_B T)^2.$$

The symmetry along the three directions implies

$$\langle p_x^2 p^4 \rangle^0 = \langle p_y^2 p^4 \rangle^0 = \langle p_z^2 p^4 \rangle^0 = \frac{1}{3} \langle p^2 p^4 \rangle^0 = \frac{1}{3} \times 105(mk_B T)^3 = 35(mk_B T)^3.$$

(c) The zeroth order approximation does not lead to relaxation of temperature/density variations related as in part (a). Find a better (time independent) approximation $f_1^1(\vec{p}, y)$, by linearizing the Boltzmann equation in the single collision time approximation, to

$$\mathcal{L}[f_1^1] \approx \left[\frac{\partial}{\partial t} + \frac{p_y}{m} \frac{\partial}{\partial y} \right] f_1^0 \approx -\frac{f_1^1 - f_1^0}{\tau_K},$$

where τ_K is of the order of the mean time between collisions.

• Since there are only variations in y , we have

$$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{p_y}{m} \frac{\partial}{\partial y} \right] f_1^0 &= f_1^0 \frac{p_y}{m} \partial_y \ln f_1^0 = f_1^0 \frac{p_y}{m} \partial_y \left[\ln n - \frac{3}{2} \ln T - \frac{p^2}{2mk_B T} - \frac{3}{2} \ln(2\pi mk_B) \right] \\ &= f_1^0 \frac{p_y}{m} \left[\frac{\partial_y n}{n} - \frac{3}{2} \frac{\partial_y T}{T} + \frac{p^2}{2mk_B T} \frac{\partial T}{T} \right] = f_1^0 \frac{p_y}{m} \left[-\frac{5}{2} + \frac{p^2}{2mk_B T} \right] \frac{\partial_y T}{T}, \end{aligned}$$

where in the last equality we have used $nT = \text{constant}$ to get $\partial_y n/n = -\partial_y T/T$. Hence the first order result is

$$f_1^1(\vec{p}, y) = f_1^0(\vec{p}, y) \left[1 - \tau_K \frac{p_y}{m} \left(\frac{p^2}{2mk_B T} - \frac{5}{2} \right) \frac{\partial_y T}{T} \right].$$

(d) Use f_1^1 , along with the averages obtained in part (b), to calculate h_y , the y component of the heat transfer vector, and hence find K , the coefficient of thermal conductivity.

• Since the velocity \vec{u} is zero, the heat transfer vector is

$$h_y = n \left\langle c_y \frac{mc^2}{2} \right\rangle^1 = \frac{n}{2m^2} \langle p_y p^2 \rangle^1.$$

In the zeroth order Gaussian weight all odd moments of p have zero average. The corrections in f_1^1 , however, give a non-zero heat transfer

$$h_y = -\tau_K \frac{n}{2m^2} \frac{\partial_y T}{T} \left\langle \frac{p_y}{m} \left(\frac{p^2}{2mk_B T} - \frac{5}{2} \right) p_y p^2 \right\rangle^0.$$

Note that we need the Gaussian averages of $\langle p_y^2 p^4 \rangle^0$ and $\langle p_y^2 p^2 \rangle^0$. From the results of part (b), these averages are equal to $35(mk_B T)^3$ and $5(mk_B T)^2$, respectively. Hence

$$h_y = -\tau_K \frac{n}{2m^3} \frac{\partial_y T}{T} (mk_B T)^2 \left(\frac{35}{2} - \frac{5 \times 5}{2} \right) = -\frac{5}{2} \frac{n\tau_K k_B^2 T}{m} \partial_y T.$$

The coefficient of thermal conductivity relates the heat transferred to the temperature gradient by $\vec{h} = -K\nabla T$, and hence we can identify

$$K = \frac{5}{2} \frac{n\tau_K k_B^2 T}{m}.$$

(e) What is the temperature profile, $T(y)$, of the gas in steady state?

• Since $\partial_t T$ is proportional to $-\partial_y h_y$, there will be no time variation if h_y is a constant. But $h_y = -K\partial_y T$, where K , which is proportional to the product nT , is a constant in the situation under investigation. Hence $\partial_y T$ must be constant, and $T(y)$ varies linearly between the two plates. Subject to the boundary conditions of $T(0) = T_1$, and $T(w) = T_2$, this gives

$$T(y) = T_1 + \frac{T_2 - T_1}{w} y.$$

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