Equilibrium in Kinetic Theory

1. *Thermalized gas particle in a one–dimensional trap:*

(a) 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

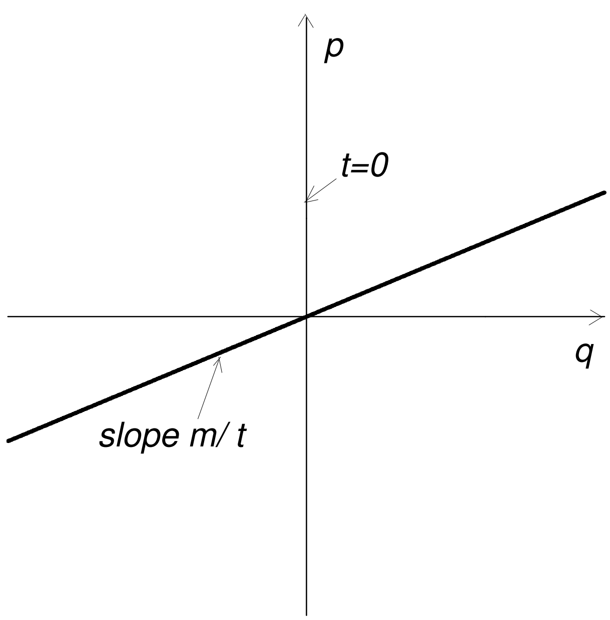
$$\mathcal{H} = \frac{p^2}{2m} + V(q_x) = \frac{p^2}{2m},$$

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

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

and hence

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

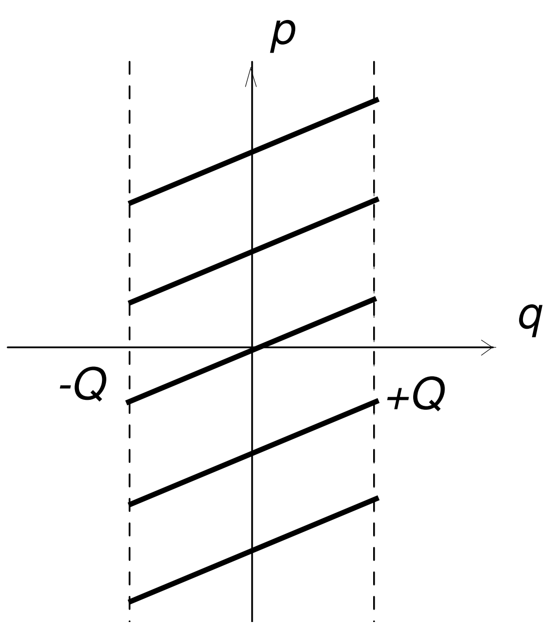
Likewise, we obtain

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

(c) 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.

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

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) 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

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

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2. *Entropy and the Ensemble Density:*

(a) A candidate "entropy" is defined by

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

Taking the derivative with respect to time gives

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

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

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

(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

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

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

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

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

Rewriting the expression for entropy,

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

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

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

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

$$\frac{\partial \rho_{max}}{\partial t} = \{ \rho_{max}, \mathcal{H} \} = \left\{ C e^{-\beta \mathcal{H}}, \mathcal{H} \right\}$$
$$= \frac{\partial \mathcal{H}}{\partial p} C(-\beta) \frac{\partial \mathcal{H}}{\partial q} e^{-\beta \mathcal{H}} - \frac{\partial \mathcal{H}}{\partial q} C(-\beta) \frac{\partial \mathcal{H}}{\partial p} e^{-\beta \mathcal{H}} = 0.$$

(d) 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.

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3. *The Vlasov equation:* The BBGKY hierarchy

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

has the characteristic time scales

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

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) 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

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

and

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

(b) 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

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

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

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

where

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

(c) 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.

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4. *Two component plasma:*

(a) 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

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

(b) 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

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

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

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

(c) Linearizing the Boltzmann weights gives

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

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

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

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) 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.

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