Physical kinetics seminar

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1.4 Liouville equation

1.4.1 The Ensemble Density in Phase Space

The state of a system at a given time is a single point in Γ-space. With time, the system point moves on the system trajectory $(q(t), p(t))$.

An ensemble is a large number of independent replicas of the same system. If there are N systems in the ensemble, then at $t=0$ The state of the ensemble is N points in Γ-space.

1.4.2 First Interpretation of $D(q,p,t)$

We now introduce the function $D(q,p,t)$. It is defined by

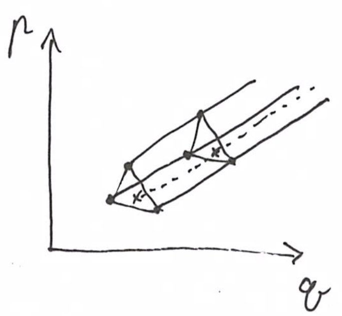
$$D(q,p,t)\,dq\,dp = D(q,p,t)\,d\Omega$$

being the number of points in the phase volume $d\Omega$ about the point (q,p) at time t. So we may write

$$D(q,p,t) = \frac{dN}{d\Omega}$$

It is important that trajectories of the ensemble never cross in Γ-space, since each trajectory is uniquely specified by $2N$ constants of motion.

From this it follows that if at some time a number of ensemble points are enclosed by a continuously closed surface, then at later times interior points remain interior, and surface points remain on the surface.



If dN is the number of enclosed points, then during the system evolution $dN \to dN' = dN$.

Lets say that $d\Omega$ is the volume of these points. Since the motion of the points is a canonical transformation, and we know from Liouville's theorem that canonical transformations leave the phase volume invariant, then $d\Omega \to d\Omega' = d\Omega$.

Combining these results we get

$$\frac{dN}{d\Omega} \to \left(\frac{dN}{d\Omega}\right)' = \frac{dN}{d\Omega}$$

Since we defined $D = \frac{dN}{d\Omega}$, we can conclude that $D(q, p, t)$ is constant on a system trajectory, or

$$\frac{dD}{dt} = 0$$

on a system trajectory. This is the Liouville equation.
Using the Poisson bracket formalism we can write

$$\frac{\partial D}{\partial t} + [D, H] = 0$$

1.4.3 Most General Solution: Second Interpretation of $D(q, p, t)$

As can be seen from the Liouville equation, a function $g(q, p, t)$ is its solution if and only if it is a constant of motion.

From this we conclude that the most general solution to the Liouville equation is an arbitrary function of all constants of motion:

$$D = D(g_1, \dots g_{2N})$$

The knowledge of the most general solution of the Liouville equation is thus equivalent to knowing all the constants of motion $g_i = g_i(q, p, t)$, $i = 1, \dots, 2N$.

Inverting the constants we obtain the dynamical orbits

$q_i = q_i(g_1, \dots, g_{2N}, t)$, $p_i = p_i(g_1, \dots, g_{2N}, t)$

Thus, the knowledge of the most general solution to the Liouville equation is equivalent to knowledge of all orbits of the system. This is the second interpretation of $D(q, p, t)$.

1.4.4 Incompressible ensemble

A second way to derive the Liouville equation is by considering ensemble flow in Γ-space.

Since system points in the ensemble are neither created nor destroyed, the rate of change of the number of points in the volume Ω (which is $\int_\Omega D \, d\Omega$) is equal to the net flux of points that pass through the closed surface S that bounds Ω.

Let $\vec{u}$ denote the velocity of system points, $\vec{u} = (\dot{q}, \dot{p})$.

Then the net flux out of the volume (reducing the number of points inside) through the closed surface S is $\oint_S \vec{u} \cdot D \, d\vec{S}$

We can then write

$$\frac{\partial}{\partial t} \int_\Omega D \, d\Omega = - \oint_S \vec{u} \cdot D \, d\vec{S} = - \int_\Omega \nabla \cdot (\vec{u} D) \, d\Omega$$

Here we used the Gauss theorem.

Thus

$$\int_\Omega d\Omega \left[\frac{\partial}{\partial t} D + \nabla \cdot (\vec{u} D) \right] = 0$$

Since the selected phase volume is arbitrary, we must have

$$\frac{\partial}{\partial t} D + \nabla \cdot (\vec{u} D) = 0$$

We have

$$\nabla \cdot (\vec{u} D) = D(\nabla \cdot \vec{u}) + (\vec{u} \cdot \nabla) D$$

Consider the first term

$$\nabla \cdot \vec{u} = \sum_i \left(\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right) = \sum_i \left(\frac{\partial^2 H}{\partial p_i \partial q_i} - \frac{\partial^2 H}{\partial q_i \partial p_i} \right) = 0$$

This implies that the fluid of the system points is incompressible. That is, along the motion trajectory the volume of the points remains constant.

Now we can consider the second term:

$$\vec{u} \cdot \nabla = \sum_i \left(\dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i} \right) = \sum_i \left(\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i} \right)$$

Thus, finally

$$\frac{\partial}{\partial t} D + (\vec{u} \cdot \nabla) D = \frac{\partial}{\partial t} D + [D, H]$$

And we obtain the same form of the Liouville equation as before.

1.4.5 Method of Characteristics

We will investigate another way of showing that the most general solution to the Liouville equation is an arbitrary function of $2N$ constants of motion.

In $2N+1$ $\tilde{\Gamma}$-space, the gradient of $D(q, p, t)$ is

$$\tilde{\nabla} D = \left(\frac{\partial D}{\partial t}, \frac{\partial D}{\partial q_1}, \dots, \frac{\partial D}{\partial p_N} \right)$$

If we introduce a vector

$$\vec{V} = \left(1, \frac{\partial H}{\partial p_1}, \dots, -\frac{\partial H}{\partial q_N} \right)$$

then we can write the Liouville equation as

$$\vec{V} \cdot \tilde{\nabla} D = 0$$

The gradient of D is normal to the vector $\vec{V}$ in $\tilde{\Gamma}$-space.
D must be a function of orbits that are tangent at every point to the vector $\vec{V}$.

Such orbits are given by solutions of

$$\frac{dt}{1} = \frac{dq_1}{\frac{\partial H}{\partial p_1}} = \dots = \frac{dp_N}{-\frac{\partial H}{\partial q_N}} \left[= \frac{dD}{0} \right]$$

These orbits are called characteristic curves.

According to the method of characteristics from the theory of linear PDE, the solution then is given by

$$\Psi(D, g_1, \dots, g_{2N}) = 0$$

$$\Rightarrow D = \phi(g_1, \dots, g_{2N})$$

With Ψ and ϕ being arbitrary functions.

So we again see that the solution of the Liouville equation is an arbitrary function of all the constants of motion.

1.4.6 Solution to the Initial-Value Problem

Taylor series expansion: Case I

We assume that we know the initial distribution (condition)

$$D(q,p,t) = D_0(q,p)$$

We expand $D(q,p,t)$ about $t=0$ at fixed values (q,p):

$$D(q,p,t) = D(q,p,0) + \frac{\partial D}{\partial t}\bigg|_{t=0} \Delta t + \frac{1}{2}\frac{\partial^2 D}{\partial t^2}\bigg|_{t=0} (\Delta t)^2 + \dots$$

From the Liouville equation we get

$$\frac{\partial D}{\partial t} = [H, D]$$

$$\frac{\partial^2 D}{\partial t^2} = \frac{\partial}{\partial t}[H, D] = \left[H, \frac{\partial D}{\partial t}\right] = [H, [H, D]]$$

Here we assumed that H does not explicitly depend on time.

Thus we obtain

$$D(q,p,t) = \left\{ 1 + \Delta t\,[H,\ ] + \frac{(\Delta t)^2}{2}[H,[H,\ ]] + \dots \right\} D_0(q,p)$$

Solution from trajectories: Case II

We assume that we know the orbits

$$q = q_0 + \tilde{q}(t), \quad p = p_0 + \tilde{p}(t)$$

and the initial distribution $D_0(q,p)$.

We have $\tilde{q}(0) = \tilde{p}(0) = 0$

The solution is based on the fact that $D(q,p,t)$ is constant along system trajectories. Thus,

$$D(q,p,t) = D_0\left(q - \tilde{q}(t), p - \tilde{p}(t)\right)$$

At $t=0$ we have $D(q,p,0) = D_0(q,p)$, so the correct initial value is reproduced.

For q, p on the system trajectory we have

$$q - \tilde{q}(t) = q_0 \quad , \quad p - \tilde{p}(t) = p_0$$

Thus on the system trajectory in $\tilde{\Gamma}$-space

$$D(q,p,t) = D_0(q_0, p_0) = \text{const}$$

So,

$$D(q,p,t) = D_0\left(q - \tilde{q}(t), p - \tilde{p}(t)\right)$$

is the solution to the Liouville equation corresponding to the initial value $D_0(q,p)$

1.4.7 Liouville operator

We introduce the Liouville operator by rewriting the Liouville equation in the form of the Schrödinger equation

$$i\frac{\partial D}{\partial t} = i[H, D] = \hat{\Lambda} D$$

Thus,

$$\hat{\Lambda} = i[H, \;] = i\sum_k \left(\frac{\partial H}{\partial q_k}\frac{\partial}{\partial p_k} - \frac{\partial H}{\partial p_k}\frac{\partial}{\partial q_k}\right)$$

Now we want to prove that $\hat{\Lambda}$ is Hermitian in space L_{2N}, which is the space of all square integrable functions of $2N$ variables. That is, $\psi(q,p)$ is an element of L_{2N} if

$$\|\psi\|^2 = \langle \psi | \psi \rangle = \int \psi^* \psi \, dq \, dp < \infty$$

An operator ~~as~~ $\hat{\Lambda}$ is Hermitian, if

$$\hat{\Lambda} = \hat{\Lambda}^+$$

with $\hat{\Lambda}^+$ being Hermitian adjoint of $\hat{\Lambda}$.

Hermitian adjoint can be described in terms of its matrix elements in $\mathcal{L}_{2N}$.

Let

$$\Lambda_{kl} = \int u_k^* \hat{\Lambda} u_l \, dq \, dp$$

where u_k and u_l are elements of a set that spans $\mathcal{L}_{2N}$.

The condition that an operator is Hermitian is written in terms of its matrix elements as

$$\Lambda_{kl} = (\Lambda_{lk})^*$$

or

$$\int u_k^* \hat{\Lambda} u_l \, dq \, dp = \int u_l \hat{\Lambda}^* u_k^* \, dq \, dp$$

Now we consider an N-body Hamiltonian

$$H = \sum_k \frac{p_k^2}{2m} + \sum_{k<l} \phi(\vec{x}_k, \vec{x}_l)$$

Here ϕ is potential of interaction between particles.

Our matrix element is

$$\Lambda_{kl} = i \int u_k^* \sum_j \left(\frac{\partial H}{\partial q_j} \frac{\partial u_l}{\partial p_j} - \frac{\partial u_l}{\partial q_j} \frac{\partial H}{\partial p_j} \right) dq \, dp$$

We have

$$u_k^* \frac{\partial u_l}{\partial p_j} = \frac{\partial}{\partial p_j}(u_k^* u_l) - u_l \frac{\partial u_k^*}{\partial p_j}$$

$$u_k^* \frac{\partial u_l}{\partial q_j} = \frac{\partial}{\partial q_j}(u_k^* u_l) - u_l \frac{\partial u_k^*}{\partial q_j}$$

We obtain

$$\Lambda_{kl} = i \int \sum_j \left\{ \frac{\partial H}{\partial q_j} \frac{\partial}{\partial p_j}(u_k^* u_l) - \frac{\partial H}{\partial q_j} u_l \frac{\partial u_k^*}{\partial p_j} - \frac{\partial}{\partial q_j}(u_k^* u_l) \frac{\partial H}{\partial p_j} + u_l \frac{\partial u_k^*}{\partial q_j} \frac{\partial H}{\partial p_j} \right\} dq \, dp$$

Because for our chosen Hamiltonian $\frac{\partial H}{\partial q_j}$ does not depend on p, we have

$$\int \frac{\partial H}{\partial q_j} \int dp_{\not{j}} \frac{\partial}{\partial p_j}(u_k^* u_l) \, dq \, dp = \int dq \int dp_{\not{j}} \frac{\partial H}{\partial q_j} (u_k^* u_l) \Big|_{p_j = -\infty}^{p_j = \infty} = 0$$

because u_k are square integrable functions.
Here $\int dp_{\not{j}} = \int dp_1 \cdots \int dp_N$ without $\int dp_j$.

We can similarly get rid of term containing $\frac{\partial}{\partial q_j}(u_k^* u_\ell)$.

We thus have

$$\Lambda_{k\ell} = i \int u_\ell \sum_j \left(- \frac{\partial H}{\partial q_j} \frac{\partial u_k^*}{\partial p_j} + \frac{\partial u_k^*}{\partial q_j} \frac{\partial H}{\partial p_j} \right) dq\, dp =$$

$$= \left[i \int u_\ell^* \sum_j \left(+ \frac{\partial H}{\partial q_j} \frac{\partial u_k}{\partial p_j} - \frac{\partial u_k}{\partial q_j} \frac{\partial H}{\partial p_j} \right) dq\, dp \right]^* =$$

$$= (\Lambda_{\ell k})^*$$

So we have proven that $\hat{\Lambda}$ is a Hermitian operator.

Therefore

- Eigenvalues of $\hat{\Lambda}$ are real
- Eigenfunctions of $\hat{\Lambda}$ are orthogonal

Note that we considered a quite general Hamiltonian, thus our conclusions are also quite general.

Also note that eigenvalues of $i\hat{\Lambda}$ will be imaginary. Thus we will have oscillating solutions. Example - sound propagation (pressure - density disturbances).