

## 3.2: Phase Flows in Classical Mechanics

### Hamiltonian evolution

The master equation provides us with a semi-phenomenological description of a dynamical system's relaxation to equilibrium. It explicitly breaks time reversal symmetry. Yet the microscopic laws of Nature are (approximately) time-reversal symmetric. How can a system which obeys Hamilton's equations of motion come to equilibrium?

Let's start our investigation by reviewing the basics of Hamiltonian dynamics. Recall the Lagrangian  $L = L(q, \dot{q}, t) = T - V$ . The Euler-Lagrange equations of motion for the action  $S[q(t)] = \int dt L$  are

$$\dot{p}_\sigma = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_\sigma} \right) = \frac{\partial L}{\partial q_\sigma}, \quad (3.2.1)$$

where  $p_\sigma$  is the canonical momentum conjugate to the generalized coordinate  $q_\sigma$ :

$$p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}. \quad (3.2.2)$$

The Hamiltonian,  $H(q, p)$  is obtained by a Legendre transformation,

$$H(q, p) = \sum_{\sigma=1}^r p_\sigma \dot{q}_\sigma - L. \quad (3.2.3)$$

Note that

$$\begin{aligned} dH &= \sum_{\sigma=1}^r \left( p_\sigma d\dot{q}_\sigma + \dot{q}_\sigma dp_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt \\ &= \sum_{\sigma=1}^r \left( \dot{q}_\sigma dp_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma \right) - \frac{\partial L}{\partial t} dt. \end{aligned}$$

Thus, we obtain Hamilton's equations of motion,

$$\frac{\partial H}{\partial p_\sigma} = \dot{q}_\sigma, \quad \frac{\partial H}{\partial q_\sigma} = -\frac{\partial L}{\partial q_\sigma} = -\dot{p}_\sigma \quad (3.2.4)$$

and

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \quad (3.2.5)$$

Define the rank  $2r$  vector  $\varphi$  by its components,

$$\varphi_i = \begin{cases} q_i & \text{if } 1 \leq i \leq r \\ p_{i-r} & \text{if } r \leq i \leq 2r. \end{cases} \quad (3.2.6)$$

Then we may write Hamilton's equations compactly as

$$\dot{\varphi}_i = J_{ij} \frac{\partial H}{\partial \varphi_j}, \quad (3.2.7)$$

where

$$J = \begin{pmatrix} 0_{r \times r} & 1_{r \times r} \\ -1_{r \times r} & 0_{r \times r} \end{pmatrix} \quad (3.2.8)$$

is a rank  $2r$  matrix. Note that  $J^t = -J$ ,  $J$  is antisymmetric, and that  $J^2 = -1_{2r \times 2r}$ .

## Dynamical systems and the evolution of phase space volumes

Consider a general dynamical system,

$$\frac{d\varphi}{dt} = \mathbf{V}(\varphi), \quad (3.2.9)$$

where  $\varphi(t)$  is a point in an  $n$ -dimensional phase space. Consider now a compact<sup>2</sup> region  $\mathcal{R}_0$  in phase space, and consider its evolution under the dynamics. That is,  $\mathcal{R}_0$  consists of a set of points  $\{\varphi \mid \varphi \in \mathcal{R}_0\}$ , and if we regard each  $\varphi \in \mathcal{R}_0$  as an initial condition, we can define the time-dependent set  $\mathcal{R}(t)$  as the set of points  $\varphi(t)$  that were in  $\mathcal{R}_0$  at time  $t = 0$ :

$$\mathcal{R}(t) = \{\varphi(t) \mid \varphi(0) \in \mathcal{R}_0\}. \quad (3.2.10)$$

Now consider the volume  $\Omega(t)$  of the set  $\mathcal{R}(t)$ . We have

$$\Omega(t) = \int_{\mathcal{R}(t)} d\mu \quad (3.2.11)$$

where

$$d\mu = d\varphi_1 d\varphi_2 \cdots d\varphi_n, \quad (3.2.12)$$

for an  $n$ -dimensional phase space. We then have

$$\Omega(t+dt) = \int_{\mathcal{R}(t+dt)} d\mu' = \int_{\mathcal{R}(t)} d\mu \left| \frac{\partial \varphi_i(t+dt)}{\partial \varphi_j(t)} \right|, \quad (3.2.13)$$

where

$$\left| \frac{\partial \varphi_i(t+dt)}{\partial \varphi_j(t)} \right| \equiv \frac{\partial(\varphi'_1, \dots, \varphi'_n)}{\partial(\varphi_1, \dots, \varphi_n)} \quad (3.2.14)$$

is a determinant, which is the Jacobean of the transformation from the set of coordinates  $\{\varphi_i = \varphi_i(t)\}$  to the coordinates  $\{\varphi'_i = \varphi_i(t+dt)\}$ . But according to the dynamics, we have

$$\varphi_i(t+dt) = \varphi_i(t) + V_i(\varphi(t)) dt + \mathcal{O}(dt^2) \quad (3.2.15)$$

and therefore

$$\frac{\partial \varphi_i(t+dt)}{\partial \varphi_j(t)} = \delta_{ij} + \frac{\partial V_i}{\partial \varphi_j} dt + \mathcal{O}(dt^2). \quad (3.2.16)$$

We now make use of the equality

$$\ln \det M = \text{Tr} \ln M, \quad (3.2.17)$$

for any matrix  $M$ , which gives us<sup>3</sup>, for small  $\varepsilon$ ,

$$\det(1 + \varepsilon A) = \exp \text{Tr} \ln(1 + \varepsilon A) = 1 + \varepsilon \text{Tr} A + \frac{1}{2} \varepsilon^2 \left( (\text{Tr} A)^2 - \text{Tr}(A^2) \right) + \dots \quad (3.2.18)$$

Thus,

$$\Omega(t+dt) = \Omega(t) + \int_{\mathcal{R}(t)} d\mu \nabla \cdot \mathbf{V} dt + \mathcal{O}(dt^2), \quad (3.2.19)$$

which says

$$\frac{d\Omega}{dt} = \int_{\mathcal{R}(t)} d\mu \nabla \cdot \mathbf{V} = \int_{\partial \mathcal{R}(t)} dS \hat{\mathbf{n}} \cdot \mathbf{V} \quad (3.2.20)$$

Here, the divergence is the *phase space divergence*,

$$\nabla \cdot \mathbf{V} = \sum_{i=1}^n \frac{\partial V_i}{\partial \varphi_i}, \quad (3.2.21)$$

and we have used the divergence theorem to convert the volume integral of the divergence to a surface integral of  $\hat{\mathbf{n}} \cdot \mathbf{V}$ , where  $\hat{\mathbf{n}}$  is the surface normal and  $dS$  is the differential element of surface area, and  $\partial \mathcal{R}$  denotes the boundary of the region  $\mathcal{R}$ . We see that if  $\nabla \cdot \mathbf{V} = 0$  everywhere in phase space, then  $\Omega(t)$  is a constant, and phase space volumes are *preserved* by the evolution of the system.

For an alternative derivation, consider a function  $\varrho(\varphi, t)$  which is defined to be the *density* of some collection of points in phase space at phase space position  $\varphi$  and time  $t$ . This must satisfy the continuity equation,

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \mathbf{V}) = 0. \quad (3.2.22)$$

This is called the *continuity equation*. It says that ‘nobody gets lost’. If we integrate it over a region of phase space  $\mathcal{R}$ , we have

$$\frac{d}{dt} \int_{\mathcal{R}} d\mu \varrho = - \int_{\mathcal{R}} d\mu \nabla \cdot (\varrho \mathbf{V}) = - \int_{\partial \mathcal{R}} dS \hat{\mathbf{n}} \cdot (\varrho \mathbf{V}). \quad (3.2.23)$$

It is perhaps helpful to think of  $\varrho$  as a charge density, in which case  $\mathbf{J} = \varrho \mathbf{V}$  is the current density. The above equation then says

$$\frac{dQ_{\mathcal{R}}}{dt} = - \int_{\partial \mathcal{R}} dS \hat{\mathbf{n}} \cdot \mathbf{J}, \quad (3.2.24)$$

where  $Q_{\mathcal{R}}$  is the total charge contained inside the region  $\mathcal{R}$ . In other words, the rate of increase or decrease of the charge within the region  $\mathcal{R}$  is equal to the total integrated current flowing in or out of  $\mathcal{R}$  at its boundary.

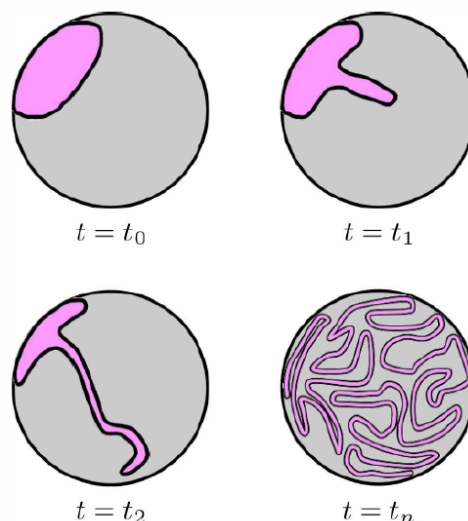


Figure 3.2.1: Time evolution of two immiscible fluids. The local density remains constant.

The Leibniz rule lets us write the continuity equation as

$$\frac{\partial \varrho}{\partial t} + \mathbf{V} \cdot \nabla \varrho + \varrho \nabla \cdot \mathbf{V} = 0. \quad (3.2.25)$$

But now suppose that the phase flow is divergenceless,  $\nabla \cdot \mathbf{V} = 0$ . Then we have

$$\frac{D\varrho}{Dt} \equiv \left( \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla \right) \varrho = 0. \quad (3.2.26)$$

The combination inside the brackets above is known as the *convective derivative*. It tells us the total rate of change of  $\varrho$  for an observer *moving with the phase flow*. That is

$$\begin{aligned}\frac{d}{dt} \varrho(\varphi(t), t) &= \frac{\partial \varrho}{\partial \varphi_i} \frac{d\varphi_i}{dt} + \frac{\partial \varrho}{\partial t} \\ &= \sum_{i=1}^n V_i \frac{\partial \varrho}{\partial \varphi_i} + \frac{\partial \varrho}{\partial t} = \frac{D\varrho}{Dt}.\end{aligned}$$

If  $D\varrho/Dt = 0$ , the local density remains the same during the evolution of the system. If we consider the ‘characteristic function’

$$\varrho(\varphi, t=0) = \begin{cases} 1 & \text{if } \varphi \in \mathcal{R}_0 \\ 0 & \text{otherwise} \end{cases} \quad (3.2.27)$$

then the vanishing of the convective derivative means that the image of the set  $\mathcal{R}_0$  under time evolution will always have the same volume.

Hamiltonian evolution in classical mechanics is volume preserving. The equations of motion are

$$\dot{q}_i = + \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = - \frac{\partial H}{\partial q_i} \quad (3.2.28)$$

A point in phase space is specified by  $r$  positions  $q_i$  and  $r$  momenta  $p_i$ , hence the dimension of phase space is  $n = 2r$ :

$$\varphi = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} \dot{\mathbf{q}} \\ \dot{\mathbf{p}} \end{pmatrix} = \begin{pmatrix} \partial H / \partial \mathbf{p} \\ -\partial H / \partial \mathbf{q} \end{pmatrix}. \quad (3.2.29)$$

Hamilton’s equations of motion guarantee that the phase space flow is divergenceless:

$$\begin{aligned}\nabla \cdot \mathbf{V} &= \sum_{i=1}^r \left\{ \frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \dot{p}_i}{\partial p_i} \right\} \\ &= \sum_{i=1}^r \left\{ \frac{\partial}{\partial q_i} \left( \frac{\partial H}{\partial p_i} \right) + \frac{\partial}{\partial p_i} \left( -\frac{\partial H}{\partial q_i} \right) \right\} = 0.\end{aligned}$$

Thus, we have that the convective derivative vanishes, viz.

$$\frac{D\varrho}{Dt} \equiv \frac{\partial \varrho}{\partial t} + \mathbf{V} \cdot \nabla \varrho = 0, \quad (3.2.30)$$

for any distribution  $\varrho(\varphi, t)$  on phase space. Thus, the value of the density  $\varrho(\varphi(t), t)$  is constant, which tells us that the phase flow is *incompressible*. In particular, phase space volumes are preserved.

### Liouville’s equation and the microcanonical distribution

Let  $\varrho(\varphi) = \varrho(\mathbf{q}, \mathbf{p})$  be a distribution on phase space. Assuming the evolution is Hamiltonian, we can write

$$\frac{\partial \varrho}{\partial t} = -\dot{\varphi} \cdot \nabla \varrho = - \sum_{k=1}^r \left( \dot{q}_k \frac{\partial}{\partial q_k} + \dot{p}_k \frac{\partial}{\partial p_k} \right) \varrho = -i \hat{L} \varrho, \quad (3.2.31)$$

where  $\hat{L}$  is a differential operator known as the *Liouvillian*:

$$\hat{L} = -i \sum_{k=1}^r \left\{ \frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} - \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} \right\}. \quad (3.2.32)$$

Equation 3.2.31, known as *Liouville’s equation*, bears an obvious resemblance to the Schrödinger equation from quantum mechanics.

Suppose that  $\Lambda_a(\varphi)$  is conserved by the dynamics of the system. Typical conserved quantities include the components of the total linear momentum (if there is translational invariance), the components of the total angular momentum (if there is rotational invariance), and the Hamiltonian itself (if the Lagrangian is not explicitly time-dependent). Now consider a distribution  $\varrho(\varphi, t) = \varrho(\Lambda_1, \Lambda_2, \dots, \Lambda_k)$  which is a function only of these various conserved quantities. Then from the chain rule, we have

$$\dot{\varphi} \cdot \nabla \varrho = \sum_a \frac{\partial \varrho}{\partial \Lambda_a} \dot{\varphi} \cdot \nabla \Lambda_a = 0, \quad (3.2.33)$$

since for each  $a$  we have

$$\frac{d\Lambda_a}{dt} = \sum_{\sigma=1}^r \left( \frac{\partial \Lambda_a}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial \Lambda_a}{\partial p_\sigma} \dot{p}_\sigma \right) = \dot{\varphi} \cdot \nabla \Lambda_a = 0 . \quad (3.2.34)$$

We conclude that any distribution  $\varrho(\varphi, t) = \varrho(\Lambda_1, \Lambda_2, \dots, \Lambda_k)$  which is a function solely of conserved dynamical quantities is a stationary solution to Liouville's equation.

Clearly the microcanonical distribution,

$$\varrho_E(\varphi) = \frac{\delta(E - H(\varphi))}{D(E)} = \frac{\delta(E - H(\varphi))}{\int d\mu \delta(E - H(\varphi))} , \quad (3.2.35)$$

is a fixed point solution of Liouville's equation.

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