Classical Liouville Equation

By: Albert Liu

Classical Phase Space Time-Evolution

Consider a classical particle moving in a well-defined potential. Given initial conditions for the position and momentum x_0 and p_0 at a time $t = 0$, which we write as a position in phase space $[x_0, p_0; 0]$, its position and momentum will evolve classically in a time Δt to definite values:

$$[x_0, p_0; 0] \xrightarrow{\Delta t} [x_{cl}(x_0, p_0, \Delta t), p_{cl}(x_0, p_0, \Delta t); \Delta t] \tag{1}$$

Just to clarify, the notation $x_{cl}(x_0, p_0, t')$ defines the position of the particle at a time $t = t'$ with the initial conditions $x = x_0$ and $p = p_0$ at $t = 0$. The meaning of $p_{cl}(x_0, p_0, t')$ is analogous.

Note that the evolution of the position and momentum in a time Δt is independent of the initial time. That is, for some arbitrary initial time $t = t'$:

$$[x_0, p_0; t'] \xrightarrow{\Delta t} [x_{cl}(x_0, p_0, \Delta t), p_{cl}(x_0, p_0, \Delta t); t' + \Delta t] \tag{2}$$

We can use this reasoning and find the evolution of position and momentum backwards in time as well, for initial conditions $x = x_0$ and $p = p_0$ at a time $t = t' + \Delta t$:

$$[x_0, p_0; t' + \Delta t] \xleftarrow{\Delta t} [x_{cl}(x_0, p_0, -\Delta t), p_{cl}(x_0, p_0, -\Delta t); t'] \tag{3}$$

Phase-Space Probability Density

This is not so useful when considering a particle with well-defined initial conditions that we know exactly. However, suppose our experimental apparatus for measuring the position and momentum is inexact, and has some uncertainty to it. In this case we can only define a phase-space probability distribution $\rho(x, p, t)$, which represents the probability density of having position and momentum values x and p at a time t. We now would like to evaluate the time-evolution of this probability distribution given its value at an initial time $t = t'$.

Note that since our particle is classical, we can use equation (3) to claim the probability of the particle having a position and momentum $x = x_{cl}(x_0, p_0, -\Delta t)$ and $p = p_{cl}(x_0, p_0, -\Delta t)]$ at an initial time $t = t'$ is equal to the probability of having a position and momentum $x = x_0$ and $p = p_0$ at a later time $t = t' + \Delta t$, since the classical evolution is deterministic. This is true for all possible values of x_0 and p_0, so we can generalize this statement to the entire phase space probability distribution:

$$\rho(x_0, p_0, t' + \Delta t) = \rho(x_{cl}(x_0, p_0, -\Delta t), p_{cl}(x_0, p_0, -\Delta t), t') \tag{4}$$

This statement is not so useful in its current form. To make progress, we Taylor expand x_{cl} and p_{cl} around $t = 0$:

$$x_{cl}(x_0, p_0, t) = x_{cl}(x_0, p_0, 0) + \dot{x}_{cl}(x_0, p_0, 0)t + \mathcal{O}(t^2) + \dots$$
$$p_{cl}(x_0, p_0, t) = p_{cl}(x_0, p_0, 0) + \dot{p}_{cl}(x_0, p_0, 0)t + \mathcal{O}(t^2) + \dots$$

Noting that $x_{cl}(x_0, p_0, 0) = x_0$ and $p_{cl}(x_0, p_0, 0) = p_0$ since there is no time-evolution, we write:

$$\begin{aligned} x_{cl}(x_0, p_0, -\Delta t) &= x_0 - \dot{x}_{cl}(x_0, p_0, 0)\Delta t + \mathcal{O}(\Delta t^2) + \dots \\ &= x_0 - \frac{\partial H}{\partial p_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots \qquad (5) \\ p_{cl}(x_0, p_0, -\Delta t) &= p_0 - \dot{p}_{cl}(x_0, p_0, 0)\Delta t + \mathcal{O}(\Delta t^2) + \dots \\ &= p_0 + \frac{\partial H}{\partial x_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots \qquad (6) \end{aligned}$$

where we used Hamilton's equations:

$$\dot{p}_{cl} = -\frac{\partial H}{\partial x_{cl}} \quad \text{and} \quad \dot{x}_{cl} = \frac{\partial H}{\partial p_{cl}} \tag{7}$$

Combining equations (4), (5), and (6), and then Taylor expanding, we find:

$$\begin{aligned} \rho(x_0, p_0, t' + \Delta t) &= \rho\left(x_0 - \frac{\partial H}{\partial p_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots, p_0 + \frac{\partial H}{\partial x_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots, t'\right) \\ &= \rho(x_0, p_0, t') + \frac{\partial \rho}{\partial x}\left(-\frac{\partial H}{\partial p_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots\right) + \frac{\partial \rho}{\partial p}\left(\frac{\partial H}{\partial x_{cl}}\Delta t + \mathcal{O}(\Delta t^2) + \dots\right) \end{aligned} \tag{8}$$

Rearranging and using the definition of a derivative:

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \lim_{\Delta t \to 0} \frac{\rho(x, p, t + \Delta t) - \rho(x, p, t)}{\Delta t} \\ &= \lim_{\Delta t \to 0} \left[-\frac{\partial H}{\partial p_{cl}}\frac{\partial \rho}{\partial x} + \frac{\partial H}{\partial x_{cl}}\frac{\partial \rho}{\partial p} + \mathcal{O}(\Delta t) + \mathcal{O}(\Delta t^2) + \dots\right] \\ &= -\frac{\partial H}{\partial p_{cl}}\frac{\partial \rho}{\partial x} + \frac{\partial H}{\partial x_{cl}}\frac{\partial \rho}{\partial p} \\ &= -i\hat{L}\rho \end{aligned} \tag{9}$$

where we've defined the Louiville operator as[1]:

$$i\hat{L} = \frac{\partial H}{\partial p_{cl}}\frac{\partial}{\partial x} - \frac{\partial H}{\partial x_{cl}}\frac{\partial}{\partial p} \tag{10}$$

[1]The factor of i in the definition for $\hat{L}$ is inserted to be analogous to the quantum Liouville equation, which governs the time-evolution of the density matrix.

This can easily be generalized to three dimensions and N particles by:

$$i\hat{L} = \sum_{j=1}^{N} \frac{\partial H}{\partial \mathbf{p}_j} \frac{\partial}{\partial \mathbf{x}_j} - \frac{\partial H}{\partial \mathbf{x}_j} \frac{\partial}{\partial \mathbf{p}_j} \tag{11}$$

where $\mathbf{x}_j$ and $\mathbf{p}_j$ refer to the position and momentum of the j^{th} particle.

Equation (11) is known as the classical Liouville equation, and has a formal solution of the form:

$$\rho(x, p, t) = e^{-i\hat{L}t} \rho(x, p, 0) \tag{12}$$

where recall, that a function of an operator is defined by its Taylor series:

$$e^{-i\hat{L}t} = \sum_{n=1}^{\infty} \frac{1}{n!} (-i\hat{L}t)^n \tag{13}$$