2.2: Liouville's Theorem for non-Hamiltonian systems

The equations of motion of a system can be cast in the generic form

$$\dot{x} = \xi(x)$$

where, for a Hamiltonian system, the vector function ξ would be

$$\xi(x) = \left(-\frac{\partial H}{\partial r_1}, \cdots, -\frac{\partial H}{\partial r_N}, \frac{\partial H}{\partial p_1}, \cdots, \frac{\partial H}{\partial p_N}\right)$$

and the incompressibility condition would be a condition on ξ:

$$\Delta_x \cdot \dot{x} = \Delta_x \cdot \xi = 0$$

A non-Hamiltonian system, described by a general vector funciton ξ, will not, in general, satisfy the incompressibility condition. That is:

$$\Delta_x \cdot \dot{x} = \Delta_x \cdot \xi \neq 0$$

Non-Hamiltonian dynamical systems are often used to describe open systems, i.e., systems in contact with heat reservoirs or mechanical pistons or particle reservoirs. They are also often used to describe driven systems or systems in contact with external fields.

The fact that the compressibility does not vanish has interesting consequences for the structure of the phase space. The Jacobian, which satisfies

$$\frac{dJ}{dt} = J\Delta_x \cdot \dot{x}$$

will no longer be 1 for all time. Defining $k = \Delta_x \cdot \dot{x}$, the general solution for the Jacobian can be written as

$$J(x_t; x_0) = J(x_0; x_0) exp\left(\int_0^t dRk(x_A)\right)$$

Note that $J(x_0; x_0) = 1$ as before. Also, note that $k = d\ln\frac{J}{dt}$. Thus, k can be expressed as the total time derivative of some function, which we will denote *W*, i.e., $k = \dot{W}$. Then, the Jacobian becomes

$$\begin{aligned} J(x_t; x_0) &= exp\left(\int_0^t dRW(x_A)\right) \\ &= exp(W(x_t) - W(x_0)) \end{aligned}$$

Thus, the volume element in phase space now transforms according to

$$dx_t = exp\left(W(x_t) - W(x_0)\right) dx_0$$

which can be arranged to read as a conservation law:

$$e^{-W(x_t)} dx_t = e^{-W(x_0)} dx_0$$

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Thus, we have a conservation law for a modified volume element, involving a "metric factor" $exp(-W(x))$. Introducing the suggestive notation $\sqrt{g} = exp(-W(x))$, the conservation law reads $\sqrt{g(x_t} dx_t = \sqrt{g(x_0} dx_0$. This is a generalized version of Liouville's theorem. Furthermore, a generalized Liouville equation for non-Hamiltonian systems can be derived which incorporates this metric factor. The derivation is beyond the scope of this course, however, the result is

$$\partial(f\sqrt{g}) + \nabla_x \cdot (\dot{x} f \sqrt{g}) = 0$$

We have called this equation, the **generalized Liouville equation** Finally, noting that $\sqrt{g}$ satisfies the same equation as *J*, i.e.,

$$\frac{d\sqrt{g}}{dt} = k\sqrt{g}$$

the presence of $\sqrt{g}$ in the generalized Liouville equation can be eliminated, resulting in

$$\frac{\partial f}{\partial t} + \dot{x} \cdot \nabla_x f = \frac{df}{dt} = 0$$

which is the ordinary Liouville equation from before. Thus, we have derived a modified version of Liouville's theorem and have shown that it leads to a conservation law for f equivalent to the Hamiltonian case. This, then, supports the generality of the Liouville equation for both Hamiltonian and non-Hamiltonian based ensembles, an important fact considering that this equation is the foundation of statistical mechanics.
