

12.3: Generalized Equations of Motion

The most general way a system can be driven away from equilibrium by a forcing function $F_e(t)$ is according to the equations of motion:

$$\dot{q}_i = \frac{\partial H}{\partial p_i} + C_i(\mathbf{x})F_e(t)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} + D_i(\mathbf{x})F_e(t)$$

where the $3N$ functions C_i and D_i are required to satisfy the incompressibility condition

$$\sum_{i=1}^{3N} \left[\frac{\partial C_i}{\partial q_i} + \frac{\partial D_i}{\partial p_i} \right] = 0$$

in order to insure that the Liouville equation for $f(\mathbf{x}, t)$ is still valid. These equations of motion will give rise to a distribution function $f(\mathbf{x}, t)$ satisfying

$$\frac{\partial f}{\partial t} + iL f = 0$$

with $\partial f / \partial t \neq 0$. (We assume that f is normalized so that $\int d\mathbf{x} f(\mathbf{x}, t) = 1$.)

What does the Liouville equation say about the nature of $f(\mathbf{x}, t)$ in the limit that C_i and D_i are small, so that the displacement away from equilibrium is, itself, small? To examine this question, we propose to solve the Liouville equation perturbatively. Thus, let us assume a solution of the form

$$f(\mathbf{x}, t) = f_0(H(\mathbf{x})) + \Delta f(\mathbf{x}, t)$$

Note, also, that the equations of motion $\dot{\mathbf{x}}$ take a perturbative form

$$\dot{\mathbf{x}}(t) = \dot{\mathbf{x}}_0 + \Delta \dot{\mathbf{x}}(t)$$

and as a result, the Liouville operator contains two pieces:

$$iL = \dot{\mathbf{x}} \cdot \nabla_{\mathbf{x}} = \dot{\mathbf{x}}_0 \cdot \nabla_{\mathbf{x}} + \Delta \dot{\mathbf{x}} \cdot \nabla_{\mathbf{x}} = iL_0 + i\Delta L$$

where $iL_0 = \{\dots, H\}$ and $f_0(H)$ is assumed to satisfy

$$iL_0 f_0(H(\mathbf{x})) = 0$$

$\dot{\mathbf{x}}_0$ means the Hamiltonian part of the equations of motion

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

For an observable $A(\mathbf{x})$, the ensemble average of A is a time-dependent quantity:

$$\langle A(t) \rangle = \int d\mathbf{x} A(\mathbf{x}) f(\mathbf{x}, t)$$

which, when the assumed form for $f(\mathbf{x}, t)$ is substituted in, gives

$$\langle A(t) \rangle = \int d\mathbf{x} A(\mathbf{x}) f_0(\mathbf{x}) + \int d\mathbf{x} A(\mathbf{x}) \Delta f(\mathbf{x}, t) = \langle A \rangle_0 + \int d\mathbf{x} A(\mathbf{x}) \Delta f(\mathbf{x}, t)$$

where $\langle \cdot \rangle_0$ means average with respect to $f_0(\mathbf{x})$.

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