6.B. The Classical Probability Density

Read §6.A of Reichl since we've skipped it in these notes.

The state of a classical N-body system is represented at each instance of time t by a point $\boldsymbol{X}^N = (\boldsymbol{q}^N, \boldsymbol{p}^N)$ in an $2\,d\,N$-D phase space Γ, where d is the spatial dimension, while $\boldsymbol{q}^N$ and $\boldsymbol{p}^N$ are the generalized coordinates and momenta, respectively.

In an experiment on a macroscopic system with $N \approx N_{\text{Avogadro}} \approx 10^{23}$, one can only specify and measure a few macroscopic properties such as pressure, temperature, etc. The exact initial conditions of the N constituent bodies are therefore never known nor desired to be known.

Classical statistical mechanics begins by assigning a probability density $\rho(\boldsymbol{X}^N, t)$ to each phase point (and hence to each possible initial conditions). The measured properties are then given by the corresponding averages over the whole phase space (and hence all possible initial conditions). Rules for assigning ρ will be discussed in the next chapter. Here, we assume ρ is known at some $t = t_0$ and explore the consequences.

A collection of identical systems with different initial conditions is called an (statistical) ensemble. The averaging discussed above is often called ensemble average.

Consider the systems represented by the points in a volume element $\Delta\Gamma$ in Γ. As they evolve, each point in $\Delta\Gamma$ will move according to the Hamiltonian equations,

$$\dot{\boldsymbol{p}}_l \equiv \frac{d\,\boldsymbol{p}_l}{d\,t} = -\frac{\partial H^N}{\partial\,\boldsymbol{q}_l} \tag{6.1}$$

$$\dot{\boldsymbol{q}}_l \equiv \frac{d\,\boldsymbol{q}_l}{d\,t} = \frac{\partial H^N}{\partial\,\boldsymbol{p}_l} \tag{6.2}$$

where $H^N(\boldsymbol{X}^N, t)$ is the Hamiltonian of the system. If H^N is time independent, the system is conservative and

$$H^N(\boldsymbol{X}^N) = E \tag{6.3}$$

where E is the (constant) total energy of the system.

In classical mechanics, a system cannot be destroyed or created during its motion. According to the theory of partial differential equations, the system paths, i.e., the solutions of (6.1-2), cover the whole phase space Γ without crossing each other. [Note: solutions can meet at essential singular points, which signify either creation or destruction of the system.] Furthermore, systems on the same trajectory differ only in the time they reach a certain reference point on the trajectory. Obviously, this time difference will be preserved as the systems evolve. Therefore, the flow of the system points is like that of a non-dissipative, incompressible fluid, i.e., $\Delta\Gamma$ can only change its shape but not its size (magnitude).

By definition, the probability of finding the system in a region $R \subset \Gamma$ at time t is

$$P(R, t) = \int_R d\,\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, t) \tag{6.5}$$

Since a system must always be somewhere in Γ,

$$\int_\Gamma d\,\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, t) = 1 \qquad \forall\ t \tag{6.4}$$

Conservation of probability means the increase of probability in a fixed R is due entirely due to the probability flow into R, i.e.,

$$\frac{d P(R,t)}{d t} = \int_R d\boldsymbol{X}^N \frac{\partial}{\partial t} \rho(\boldsymbol{X}^N, t)$$
$$= -\oint_S dS\, \hat{\boldsymbol{s}}^N \cdot \dot{\boldsymbol{X}}^N \rho(\boldsymbol{X}^N, t) \tag{6.6}$$

where $\hat{\boldsymbol{s}}^N$ is the outward unit normal to the surface S enclosing R.

Using the Gauss's theorem to change the surface integral into a volume one, (6.6) becomes

$$\int_R d\boldsymbol{X}^N \frac{\partial}{\partial t} \rho(\boldsymbol{X}^N, t) = -\int_R d\boldsymbol{X}^N \nabla_{\boldsymbol{X}^N} \cdot \left[\dot{\boldsymbol{X}}^N \rho(\boldsymbol{X}^N, t)\right] \tag{6.7}$$

where

$$\nabla_{\boldsymbol{X}^N} = (\nabla_{\boldsymbol{q}^N}, \nabla_{\boldsymbol{p}^N}) = \left(\frac{\partial}{\partial \boldsymbol{q}_1}, \ldots \frac{\partial}{\partial \boldsymbol{q}_N}, \frac{\partial}{\partial \boldsymbol{p}_1}, \ldots \frac{\partial}{\partial \boldsymbol{p}_N}\right) \tag{6.7a}$$

is the gradient operator in Γ.

Since (6.7) is valid for any R, we have

$$\frac{\partial}{\partial t} \rho(\boldsymbol{X}^N, t) + \nabla_{\boldsymbol{X}^N} \cdot \left[\dot{\boldsymbol{X}}^N \rho(\boldsymbol{X}^N, t)\right] = 0 \tag{6.8}$$

which is the balance equation, or equation of continuity, for ρ in Γ.

The evolution of a phase space volume element $d\boldsymbol{X}^N(t_0) \to d\boldsymbol{X}^N(t)$ can be viewed as a coordinate transformation $\boldsymbol{X}^N(t_0) \to \boldsymbol{X}^N(t)$ so that

$$d\boldsymbol{X}^N(t) = \mathcal{J}^N(t, t_0)\, d\boldsymbol{X}^N(t_0) \tag{6.9}$$

where the Jacobian of the transformation is given by

$$\mathcal{J}^N(t, t_0) = \det\left|\frac{\partial \boldsymbol{X}^N(t)}{\partial \boldsymbol{X}^N(t_0)}\right| = \det\begin{vmatrix} \frac{\partial \boldsymbol{q}^N(t)}{\partial \boldsymbol{q}^N(t_0)} & \frac{\partial \boldsymbol{q}^N(t)}{\partial \boldsymbol{p}^N(t_0)} \\ \frac{\partial \boldsymbol{p}^N(t)}{\partial \boldsymbol{q}^N(t_0)} & \frac{\partial \boldsymbol{p}^N(t)}{\partial \boldsymbol{p}^N(t_0)} \end{vmatrix} \tag{6.10}$$

For the transformations

$$\boldsymbol{X}^N(t_0) \to \boldsymbol{X}^N(t_1) \to \boldsymbol{X}^N(t)$$

we have

$$d\boldsymbol{X}^N(t_1) = \mathcal{J}^N(t_1, t_0)\, d\boldsymbol{X}^N(t_0)$$
$$d\boldsymbol{X}^N(t) = \mathcal{J}^N(t, t_1)\, d\boldsymbol{X}^N(t_1) = \mathcal{J}^N(t, t_1)\, \mathcal{J}^N(t_1, t_0)\, d\boldsymbol{X}^N(t_0)$$
$$= \mathcal{J}^N(t, t_0)\, d\boldsymbol{X}^N(t_0)$$

$$\therefore \quad \mathcal{J}^N(t, t_0) = \mathcal{J}^N(t, t_1)\, \mathcal{J}^N(t_1, t_0) \tag{6.11}$$

For a short time transition with $\Delta t = t - t_0 \to 0$,

$$\boldsymbol{X}^N(t + \Delta t) = \boldsymbol{X}^N(t) + \dot{\boldsymbol{X}}^N(t)\, \Delta t + O(\Delta t)^2$$

or

$$\boldsymbol{q}^N(t + \Delta t) = \boldsymbol{q}^N(t) + \dot{\boldsymbol{q}}^N(t)\, \Delta t + O(\Delta t)^2 \tag{6.13}$$
$$\boldsymbol{p}^N(t + \Delta t) = \boldsymbol{p}^N(t) + \dot{\boldsymbol{p}}^N(t)\, \Delta t + O(\Delta t)^2 \tag{6.12}$$

$$\to \quad \mathcal{J}^N(t + \Delta t, t) = \det\begin{vmatrix} 1 + \frac{\partial \dot{\boldsymbol{q}}^N(t)}{\partial \boldsymbol{q}^N(t)} \Delta t & \frac{\partial \boldsymbol{q}^N(t)}{\partial \boldsymbol{p}^N(t)} \Delta t \\ \frac{\partial \boldsymbol{p}^N(t)}{\partial \boldsymbol{q}^N(t)} \Delta t & 1 + \frac{\partial \dot{\boldsymbol{p}}^N(t)}{\partial \boldsymbol{p}^N(t)} \Delta t \end{vmatrix} + O(\Delta t)^2$$
$$= 1 + \left(\frac{\partial \dot{\boldsymbol{q}}^N}{\partial \boldsymbol{q}^N} + \frac{\partial \dot{\boldsymbol{p}}^N}{\partial \boldsymbol{p}^N}\right)_t \Delta t + O(\Delta t)^2 \tag{6.14}$$

Using (6.1-2), we have

$$\frac{\partial \dot{\boldsymbol{q}}^N}{\partial \boldsymbol{q}^N} + \frac{\partial \dot{\boldsymbol{p}}^N}{\partial \boldsymbol{p}^N} = \frac{\partial^2 H^N}{\partial \boldsymbol{q}^N \partial \boldsymbol{p}^N} - \frac{\partial H^N}{\partial \boldsymbol{p}^N \partial \boldsymbol{q}^N} = 0 \tag{6.15}$$

so that (6.14) becomes

$$\mathcal{J}^N(t+\Delta t, t) = 1 + O(\Delta t)^2 \tag{6.16}$$

with

$$\mathcal{J}^N(t, t) = 1$$

On the other hand, (6.11) gives

$$\mathcal{J}^N(t+\Delta t, t_0) = \mathcal{J}^N(t+\Delta t, t)\,\mathcal{J}^N(t, t_0) \qquad \forall\ t_0$$

Hence,

$$\begin{aligned}\frac{d\,\mathcal{J}^N(t, t_0)}{d t} &\equiv \lim_{\Delta t\to 0} \frac{\mathcal{J}^N(t+\Delta t,\ t_0) - \mathcal{J}^N(t, t_0)}{\Delta t} \\ &= \lim_{\Delta t\to 0} \frac{\mathcal{J}^N(t+\Delta t, t)\,\mathcal{J}^N(t, t_0) - \mathcal{J}^N(t, t_0)}{\Delta t} \\ &= \lim_{\Delta t\to 0} \frac{\left[1 + O(\Delta t)^2\right]\mathcal{J}^N(t, t_0) - \mathcal{J}^N(t, t_0)}{\Delta t} \\ &= \lim_{\Delta t\to 0} O(\Delta t) \\ &= 0 \qquad \forall\ t_0 \end{aligned} \tag{6.18}$$

$$\begin{aligned}\therefore \qquad \mathcal{J}^N(t, t_0) &= \text{const} && \forall\ t,\ t_0 \\ &= 1 && [\ (6.16) \text{ used. }] \end{aligned} \tag{6.19}$$

(6.9) thus simplifies to

$$d\,\boldsymbol{X}^N(t) = d\,\boldsymbol{X}^N(t_0) \tag{6.20}$$

thus supporting our previous claim that $\Delta\Gamma$ does not change size as the systems represented by it evolve.

Furthermore, (6.15) can be written as

$$\nabla_{\boldsymbol{X}^N}\cdot\dot{\boldsymbol{X}}^N = \frac{\partial\,\dot{\boldsymbol{q}}^N}{\partial\,\boldsymbol{q}^N} + \frac{\partial\,\dot{\boldsymbol{p}}^N}{\partial\,\boldsymbol{p}^N} = 0 \tag{6.21}$$

which is the mathematical statement that the probability flow is incompressible.

The equation of continuity (6.8) thus simplifies to

$$\frac{\partial}{\partial t}\rho\left(\boldsymbol{X}^N, t\right) + \dot{\boldsymbol{X}}^N\cdot\nabla_{\boldsymbol{X}^N}\rho\left(\boldsymbol{X}^N, t\right) = 0 \tag{6.22}$$

$$= \frac{d\,\rho\left(\boldsymbol{X}^N, t\right)}{d t} \tag{6.24}$$

where

$$\frac{d}{d t} = \frac{\partial}{\partial t} + \dot{\boldsymbol{X}}^N\cdot\nabla_{\boldsymbol{X}^N} \tag{6.23}$$

is the total (or convective) time derivative.

Thus, ρ is a constant in the neighborhood of an observer moving with the probability fluid.

Using (6.1-2), we can also write

$$\begin{aligned}\dot{\boldsymbol{X}}^N\cdot\nabla_{\boldsymbol{X}^N} &= \dot{\boldsymbol{q}}^N\cdot\frac{\partial}{\partial\,\boldsymbol{q}^N} + \dot{\boldsymbol{p}}^N\cdot\frac{\partial}{\partial\,\boldsymbol{p}^N} \\ &= \frac{\partial H^N}{\partial\,\boldsymbol{p}^N}\cdot\frac{\partial}{\partial\,\boldsymbol{q}^N} - \frac{\partial H^N}{\partial\,\boldsymbol{q}^N}\cdot\frac{\partial}{\partial\,\boldsymbol{p}^N} \qquad [\text{c.f. } (6.15)] \\ &= -\left\{ H^N,\ \right\}_{\boldsymbol{q},\boldsymbol{p}} \\ &\equiv \hat{\mathcal{H}}^N \end{aligned} \tag{6.26}$$

where the Poisson bracket is defined as

$$\{A, B\}_{\boldsymbol{q},\boldsymbol{p}} = \frac{\partial A}{\partial \boldsymbol{q}^N} \cdot \frac{\partial B}{\partial \boldsymbol{p}^N} - \frac{\partial B}{\partial \boldsymbol{q}^N} \cdot \frac{\partial A}{\partial \boldsymbol{p}^N} = \sum_{j=1}^{N} \left(\frac{\partial A}{\partial \boldsymbol{q}_j} \cdot \frac{\partial B}{\partial \boldsymbol{p}_j} - \frac{\partial B}{\partial \boldsymbol{q}_j} \cdot \frac{\partial A}{\partial \boldsymbol{p}_j} \right)$$

(6.22) thus simplifies to

$$\frac{\partial \rho}{\partial t} = -\hat{\mathcal{H}}^N \rho = \{ H^N, \rho \}_{\boldsymbol{q},\boldsymbol{p}} \tag{6.25}$$

(6.25) is often written as

$$i \frac{\partial \rho}{\partial t} = \hat{L}^N \rho \tag{6.27}$$

where

$$\hat{L}^N = -i \hat{\mathcal{H}}^N$$

is the Liouville operator and (6.27) is known as the Liouville equation.

For a time-independent H^N, the solution to (6.27) is

$$\rho(\boldsymbol{X}^N, t) = e^{-it\hat{L}^N} \rho(\boldsymbol{X}^N, 0) \tag{6.28}$$

For a stationary solution,

$$\frac{\partial \rho^s(\boldsymbol{X}^N)}{\partial t} = 0 \qquad \to \qquad \hat{L}^N \rho^s(\boldsymbol{X}^N) = 0 \tag{6.29}$$

See Reichl's comments on p.292.

Exercise 6.1.

Consider a particle that bounces elastically and vertically off the floor under the influence of gravity and no friction. At time $t = 0$, the particle is on the floor at $z = 0$ and has upward momentum $p = p_0$. Its maximum height is at $z = h$.

Solve the Liouville equation to find the probability density $\rho(z, p, t)$.

Answer

Since there is only one set of initial conditions, we known exactly where the phase point of the particle is at all times. ρ is therefore a 2-D delta function that is non-zero only its path.

The Hamiltonian of the particle is

$$H = \frac{1}{2m} p^2 + V(z) \qquad \text{with} \qquad V(z) = \begin{cases} m g z & z \geq 0 \\ \infty & z < 0 \end{cases}$$

In the absence of friction, the particle will fall & bounds back repeatedly. The motion is therefore periodic and its path in the z-p phase space is closed.

The property $V(z) = \infty \; \forall \; z < 0$ can be enforced by the condition

$$p(n T) = p_0 \qquad n = 0, 1, 2, \ldots \tag{1a}$$

where T is the period of the motion.

At the end points $z = 0$ & $z = h$, we have

$$E = \frac{1}{2m} p^2(nT) = \frac{1}{2m} p_0^2 \qquad \& \qquad E = V(h) = m g h$$

$$\rightarrow \qquad p_0 = m\sqrt{2 g h}$$

The Hamilton's equations are

$$\dot{z} = \frac{\partial H}{\partial p} = \frac{p}{m} \qquad \& \qquad \dot{p} = -\frac{\partial H}{\partial z} = -m g \tag{1b}$$

Integrating, we have

$$p(t + nT) = p(nT) - m g t = m\sqrt{2 g h} - m g t \tag{1c}$$

$$z(t + nT) = \frac{1}{m}\int_0^t d t\, p(t + nT) = \sqrt{2 g h}\, t - \frac{1}{2} g t^2 \tag{1}$$

Setting $t = T$ in (1), we have

$$0 = \sqrt{2 g h}\, T - \frac{1}{2} g T^2$$

$$\rightarrow \qquad T = 2\sqrt{\frac{2h}{g}} \tag{1d}$$

Note that using (1c) to calculate T is more tricky owing to (1a). In fact, setting $t = T$ in (1c) gives

$$p[(n+1)T] = p(nT) - m g T$$

$$= m\sqrt{2 g h} - m g T \qquad \text{[(1a) used.]}$$

$$= -m\sqrt{2 g h} \qquad \text{[(1d) used.]}$$

which contradicts (1a). This is acceptable since, to begin the next cycle, the elastic collision with the ground will add $2m\sqrt{2 g h}$ to p so that (1a) is again satisfied.

A better way to describe periodic motion in phase space is to switch to the action-angle variables. The action is defined as

$$J = \oint d z\, p \tag{2a}$$

Note the extra factor of $\frac{1}{2\pi}$ in Reichl's definition. Thus,

$$J_{\text{Reichl}} = \frac{1}{2\pi} J \tag{2b}$$

Combining the two equations in (1b) gives

$$\frac{d p}{d z} = -\frac{m^2 g}{p}$$

$$\rightarrow \qquad \frac{1}{2} p^2 = \frac{1}{2} p_0^2 - m^2 g z = m E - m^2 g z$$

$$\therefore \qquad p = \pm\sqrt{2m(E - m g z)}$$

Thus,

$$J = \int_0^h d z\sqrt{2m(E - m g z)} + \int_h^0 d z\left(-\sqrt{2m(E - m g z)}\right)$$

$$= 2\sqrt{2m}\int_0^h d z\sqrt{E - m g z}$$

$$= 2\sqrt{2m^2 g}\int_0^h d z\sqrt{h - z} \qquad (E = m g h)$$

$$= 2\sqrt{2m^2 g}\ \frac{2}{3} h^{3/2} \tag{2c}$$

$$= \frac{4}{3}\sqrt{2m^2 g}\left(\frac{E}{m g}\right)^{3/2} = \frac{4}{3g}\sqrt{\frac{2}{m}}\ E^{3/2} \tag{2}$$

$$\rightarrow \qquad E = \left(\frac{3g}{4}\right)^{2/3}\left(\frac{m}{2}\right)^{1/3} J^{2/3}$$

$$= \left(\frac{9g^2 m}{32}\right)^{1/3} J^{2/3} = H \tag{3}$$

Hence,

$$\dot{J} = -\frac{\partial H}{\partial \theta} = 0$$

so that J is a constant of the motion.

$$\dot{\theta} = \frac{\partial H}{\partial J}$$

$$= \frac{2}{3}\left(\frac{9g^2 m}{32}\right)^{1/3} J^{-1/3} = \left(\frac{g^2 m}{12J}\right)^{1/3} \qquad \text{[(3) used.]} \tag{4a}$$

$$= \frac{g}{2}\sqrt{\frac{m}{2E}} \qquad \text{[(2) used.]}$$

$$= \frac{1}{2}\sqrt{\frac{g}{2h}} \qquad [\ E = m g h\ ]$$

$$= \frac{1}{T} \qquad \text{[(1d) used.]}$$

$$\equiv \frac{\omega}{2\pi} \tag{4}$$

$$\rightarrow \qquad \theta(t) = \theta(0) + \frac{\omega}{2\pi} t \tag{4b}$$

Thus,

$$\theta_{\text{Reichl}} = 2\pi\theta \tag{4c}$$

(2b) & (4c) can be used to convert our results with Reichl's. Note that

$$\theta_{\text{Reichl}} J_{\text{Reichl}} = \theta J \qquad \rightarrow \qquad d\theta_{\text{Reichl}}\, dJ_{\text{Reichl}} = d\theta\, dJ$$

For the sake of simplicity, we set $\theta(0) = 0$ so that

$$t = \frac{2\pi}{\omega}\theta$$

$$= \left(\frac{12}{g^2 m} J\right)^{1/3} \theta \qquad \text{[(4a) used.]}$$

Putting this into (1c) & (1) gives

$$p = m\sqrt{2gh} - m g\left(\frac{12}{g^2 m} J\right)^{1/3} \theta$$

$$z = \sqrt{2gh}\left(\frac{12}{g^2 m} J\right)^{1/3} \theta - \frac{1}{2} g\left(\frac{12}{g^2 m} J\right)^{2/3} \theta^2$$

Inverting (2c) gives

$$h = \frac{1}{2}\left(\frac{3}{2\sqrt{m^2 g}} J\right)^{2/3} \qquad \to \qquad \sqrt{2 g h} = \left(\frac{3 g}{2 m} J\right)^{1/3}$$

Hence,

$$p = m\left(\frac{3 g}{2 m} J\right)^{1/3} - m g\left(\frac{12}{g^2 m} J\right)^{1/3} \theta$$

$$= m\left(\frac{3 g}{2 m} J\right)^{1/3} (1 - 2\theta) \qquad (5a)$$

$$z = \left(\frac{3 g}{2 m} J\right)^{1/3} \left(\frac{12}{g^2 m} J\right)^{1/3} \theta - \frac{1}{2} g \left(\frac{12}{g^2 m} J\right)^{2/3} \theta^2$$

$$= \frac{2}{g}\left(\frac{3 g}{2 m} J\right)^{2/3} (\theta - \theta^2) \qquad (5)$$

Setting

$$a = m\left(\frac{3 g}{2 m}\right)^{1/3} \qquad b = \frac{2}{g}\left(\frac{3 g}{2 m}\right)^{2/3} = \frac{2 a^2}{m^2 g}$$

we have

$$p = a J^{1/3}(1 - 2\theta) \qquad z = b J^{2/3}(\theta - \theta^2) \qquad (5b)$$

(5b) describes the transformation between the two sets of phase space variables (z, p) & (θ, J).
Setting

$$d z\, d p = \mathcal{J}\, d\theta\, d J$$

we have

$$\mathcal{J} = \det \begin{vmatrix} \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial J} \\ \frac{\partial p}{\partial \theta} & \frac{\partial p}{\partial J} \end{vmatrix}$$

$$= \det \begin{vmatrix} b J^{2/3}(1 - 2\theta) & \frac{2}{3} b J^{-1/3}(\theta - \theta^2) \\ -2 a J^{1/3} & \frac{1}{3} a J^{-2/3}(1 - 2\theta) \end{vmatrix}$$

$$= \frac{1}{3} a b (1 - 2\theta)^2 + \frac{4}{3} a b (\theta - \theta^2)$$

$$= \frac{1}{3} a b = \frac{2 a^3}{3 m^2 g} = 1$$

$$\to \qquad d z\, d p = d\theta\, d J$$

The Liouville equation (6.22) thus takes the form

$$\frac{\partial \rho}{\partial t} + \dot{z}\frac{\partial \rho}{\partial z} + \dot{p}\frac{\partial \rho}{\partial p} = 0 \qquad \rho = \rho(z, p, t) \qquad (7)$$

or

$$\frac{\partial \rho'}{\partial t} + \dot{\theta}\frac{\partial \rho'}{\partial \theta} = 0 \qquad \rho' = \rho'(\theta, J, t) \qquad (8)$$

The initial conditions

$$z(0) = 0 p(0) = p_0$$

correspond to

$$J(0) = J_0$$

$$= \frac{4}{3g}\sqrt{\frac{2}{m}}\left(\frac{p_0^2}{2m}\right)^{3/2} \qquad \text{[(2) used.]}$$
$$= 2\sqrt{2m^2 g}\;\frac{2}{3}h^{3/2} \qquad \text{[(2c) used.]}$$

while we have previously agreed to set

$$\theta(0) = 0$$

Thus,

$$\rho(z, p, 0) = \delta(z)\,\delta(p - p_0)$$
$$\rho'(\theta, J, 0) = \delta(\theta)\,\delta(J - J_0)$$

Since J is a constant of motion, while $\theta(t)$ is given by (4b), we have

$$\rho'(\theta, J, t) = \delta(\theta - \omega t)\,\delta(J - J_0) \qquad (12)$$

where

$$\omega = 2\pi\left(\frac{g^2 m}{12 J_0}\right)^{1/3} \qquad \text{[(4a) used.]}$$

(5a) & (5) can be written as

$$p(J_0, \omega t) = m\left(\frac{3g}{2m}J_0\right)^{1/3}(1 - 2\omega t)$$
$$z(J_0, \omega t) = \frac{2}{g}\left(\frac{3g}{2m}J_0\right)^{2/3}(\omega t - \omega^2 t^2)$$

so that

$$\rho(z, p, t) = \delta\big(z - z(J_0, \omega t)\big)\,\delta\big(p - p(J_0, \omega t)\big) \qquad (13)$$

Since the motion is periodic with period $T = \frac{2\pi}{\omega}$, so is ρ'. This can be shown explicitly using the delta function expansion

$$\delta(\theta - \omega t) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} e^{in(\theta - \omega t)}$$

so that (12) becomes

$$\rho'(\theta, J, t) = \delta(J - J_0)\,\frac{1}{2\pi}\sum_{n=-\infty}^{\infty} e^{in(\theta - \omega t)}$$

which shows that ρ' is also periodic in θ with period 2π. Furthermore, we can write

$$\rho'(\theta, J, t) = \frac{1}{2\pi}\sum_{m,n=-\infty}^{\infty}\frac{e^{im(J - J_0)}}{2\pi}e^{in(\theta - \omega t)}$$
$$= \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\tilde{\rho}_n(J, 0)\,e^{in(\theta - \omega t)} \qquad (11)$$
$$= \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\tilde{\rho}_n(J, t)\,e^{in\theta} \qquad (9)$$

where

$$\tilde{\rho}_n(J, 0) = \frac{1}{2\pi}\sum_{m(\neq n)=-\infty}^{\infty} e^{im(J - J_0)}$$
$$\tilde{\rho}_n(J, t) = \tilde{\rho}_n(J, 0)\,e^{-in\omega t} = \frac{1}{2\pi}\sum_{m(\neq n)=-\infty}^{\infty} e^{im(J - J_0) - in\omega t} \qquad (10)$$

Expectation Values

The expectation value of a phase space function $O^N(\boldsymbol{X}^N)$ at time t is defined as

$$\begin{aligned}\langle O(t)\rangle &= \int d\boldsymbol{X}^N\, O^N(\boldsymbol{X}^N)\,\rho(\boldsymbol{X}^N, t)\\ &= \int d\boldsymbol{X}^N\, O^N(\boldsymbol{X}^N)\, e^{-i t \hat{L}^N}\,\rho(\boldsymbol{X}^N, 0)\end{aligned} \tag{6.30}$$

where

$$d\boldsymbol{X}^N = d\boldsymbol{X}_1 \cdots d\boldsymbol{X}_N$$

Taylor expansion of $e^{-i t \hat{L}^N}$ gives

$$\langle O(t)\rangle = \int d\boldsymbol{X}^N\, O^N(\boldsymbol{X}^N) \sum_{n=0}^{\infty} \frac{(-i t)^n}{n!} (\nabla_{\boldsymbol{X}^N})^n\,\rho(\boldsymbol{X}^N, 0)$$

Assuming $\rho\left(\boldsymbol{X}^N, 0\right)\Big|_{|\boldsymbol{X}|^N \to \infty} = 0$, partial integrating n times for the n^{th} term gives

$$\begin{aligned}\langle O(t)\rangle &= \int d\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, 0) \sum_{n=0}^{\infty} (-)^n \frac{(-i t)^n}{n!} (\nabla_{\boldsymbol{X}^N})^n\, O^N(\boldsymbol{X}^N)\\ &= \int d\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, 0) \sum_{n=0}^{\infty} \frac{(i t)^n}{n!} (\nabla_{\boldsymbol{X}^N})^n\, O^N(\boldsymbol{X}^N)\\ &= \int d\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, 0)\, e^{i t \hat{L}^N}\, O^N(\boldsymbol{X}^N)\\ &= \int d\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, 0)\, e^{i t \hat{L}^N}\, O^N(\boldsymbol{X}^N, 0)\\ &= \int d\boldsymbol{X}^N\,\rho(\boldsymbol{X}^N, 0)\, O^N(\boldsymbol{X}^N, t)\end{aligned} \tag{6.31}$$

where

$$O^N(\boldsymbol{X}^N, t) = e^{i t \hat{L}^N}\, O^N(\boldsymbol{X}^N, 0) \tag{6.31a}$$

with

$$O^N(\boldsymbol{X}^N, 0) = O^N(\boldsymbol{X}^N)$$

defines the “Heisenberg picture” in which the phase functions $O^N(\boldsymbol{X}^N, t)$ carry the evolution information, as opposed to the “Schrodinger picture” used in (6.30) where the task is assumed by the state (probability) density $\rho(\boldsymbol{X}^N, t)$.

(6.31a) gives

$$i \frac{\partial}{\partial t} O^N(\boldsymbol{X}^N, t) = -\hat{L}^N\, O^N(\boldsymbol{X}^N, t) \tag{6.32}$$

which replaces the Liouville equation (6.27).

Exercise 6.2.

A system of N particles has a Hamiltonian

$$\begin{aligned}H &= \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{j=1}^{N} \sum_{i=1}^{j-1} V(\,|\,\boldsymbol{q}_i - \boldsymbol{q}_j\,|\,)\\ &= \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{i<j}^{N(N-1)/2} V(\,|\,\boldsymbol{q}_i - \boldsymbol{q}_j\,|\,)\end{aligned}$$

which contains $C_2^N = \frac{1}{2} N(N-1)$ pair-wise inter-particle interactions.

The phase function which gives the particle density at position $\boldsymbol{R}$ in configuration space is

$$n(\boldsymbol{q}^N, \boldsymbol{R}) = \sum_{i=1}^{N} \delta(\boldsymbol{q}_i - \boldsymbol{R})$$

Write the equation of motion for $n(\boldsymbol{q}^N, \boldsymbol{R})$.

Answer

Using (6.26), we have

$$\begin{aligned}
\hat{L}^N = -i\,\hat{H}^N &= -i \sum_{i=1}^{N} \left(\frac{\partial H}{\partial \boldsymbol{p}_i} \cdot \frac{\partial}{\partial \boldsymbol{q}_i} - \frac{\partial H}{\partial \boldsymbol{q}_i} \cdot \frac{\partial}{\partial \boldsymbol{p}_i} \right) \\
&= -i \sum_{i=1}^{N} \left(\frac{\boldsymbol{p}_i}{m} \cdot \frac{\partial}{\partial \boldsymbol{q}_i} - \frac{\partial H}{\partial \boldsymbol{q}_i} \cdot \frac{\partial}{\partial \boldsymbol{p}_i} \right) \\
&= -i \sum_{i=1}^{N} \left(\dot{\boldsymbol{q}}_i \cdot \frac{\partial}{\partial \boldsymbol{q}_i} - \frac{\partial H}{\partial \boldsymbol{q}_i} \cdot \frac{\partial}{\partial \boldsymbol{p}_i} \right)
\end{aligned}$$

(6.32) then gives

$$\begin{aligned}
\frac{\partial n}{\partial t} &= i\,\hat{L}^N n \\
&= \sum_{i=1}^{N} \dot{\boldsymbol{q}}_i \cdot \frac{\partial}{\partial \boldsymbol{q}_i} \sum_{j=1}^{N} \delta(\boldsymbol{q}_j - \boldsymbol{R}) \\
&= \sum_{i=1}^{N} \dot{\boldsymbol{q}}_i \cdot \frac{\partial}{\partial \boldsymbol{q}_i} \delta(\boldsymbol{q}_i - \boldsymbol{R}) && (1) \\
&= -\sum_{i=1}^{N} \dot{\boldsymbol{q}}_i \cdot \nabla_{\boldsymbol{R}}\, \delta(\boldsymbol{q}_i - \boldsymbol{R}) \\
&= -\nabla_{\boldsymbol{R}} \cdot \sum_{i=1}^{N} \dot{\boldsymbol{q}}_i\, \delta(\boldsymbol{q}_i - \boldsymbol{R}) \\
&= -\nabla_{\boldsymbol{R}} \cdot \sum_{i=1}^{N} \frac{\boldsymbol{p}_i}{m} \delta(\boldsymbol{q}_i - \boldsymbol{R}) && (2) \\
&= -\nabla_{\boldsymbol{R}} \cdot \boldsymbol{J}(\boldsymbol{q}^N, \boldsymbol{p}^N; \boldsymbol{R}) && (3)
\end{aligned}$$

where

$$\boldsymbol{J}(\boldsymbol{q}^N, \boldsymbol{p}^N; \boldsymbol{R}) = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i}{m} \delta(\boldsymbol{q}_i - \boldsymbol{R}) = \sum_{i=1}^{N} \dot{\boldsymbol{q}}_i\, \delta(\boldsymbol{q}_i - \boldsymbol{R})$$

is the particle current density at $\boldsymbol{R}$.