APPENDIX G

Hamiltonian Formulation of Classical Mechanics

In this appendix, we briefly review some aspects of the Hamiltonian formulation of classical mechanics. The Hamiltonian function for a single particle described by a single coordinate, call it x, is a function of x and the so-called "conjugate momentum," p_x. Examples of such coordinate pairs include

- x and $p_x = m\dot{x}$ (ordinary momentum) for translational motion and
- θ and $p_\theta = L_z = mr^2\dot{\theta}$ (angular momentum) for a rotational system.

The Hamiltonian is written as $H = H(x, p_x)$ and x and p_x are initially considered as independent variables.

The dynamical equations of motion for $x(t)$ and $p_x(t)$ are *Hamilton's equations*, namely

$$\frac{dx}{dt} = \dot{x} = \frac{\partial H}{\partial p_x} \tag{G.1}$$

$$-\frac{dp_x}{dt} = -\dot{p}_x = \frac{\partial H}{\partial x} \tag{G.2}$$

To see the equivalence to Newtonian mechanics, note that the Hamiltonian function

$$H(x, p_x) = \frac{p_x^2}{2m} + V(x) \tag{G.3}$$

gives the equations

$$\dot{x} = \frac{p_x}{m} \quad \text{and} \quad -\dot{p}_x = \frac{\partial V(x)}{\partial x} \equiv -F(x) \tag{G.4}$$

or

$$m\ddot{x} = \dot{p}_x = F(x) \tag{G.5}$$

The Hamiltonian function for the degrees of freedom of more than one particle (in one dimension) can be written

$$H = H(x_i, p_i) = \sum_i \frac{p_i^2}{2m_i} + \sum_i V_i(x_i) + \sum_{i>j} V_{ij}(x_i - x_j) \tag{G.6}$$

with the corresponding equations

$$\frac{dx_i}{dt} = \dot{x}_i = \frac{\partial H}{\partial p_i} \tag{G.7}$$

$$-\frac{dp_i}{dt} = -\dot{p}_i = \frac{\partial H}{\partial x_i} \tag{G.8}$$

For two functions which depend on the coordinates of a multivariable problem (and possibly the time coordinate explicitly), $g = g(x_i, p_i; t)$ and $h = h(x_i, p_i; t)$, the *Poisson bracket* is defined via

$$[g, h] = \sum_k \left(\frac{\partial g}{\partial x_k} \frac{\partial h}{\partial p_k} - \frac{\partial g}{\partial p_k} \frac{\partial h}{\partial x_k} \right) \tag{G.9}$$

Any such arbitrary function can depend on time either from an explicit t dependence or via the coordinates $x_i(t), p_i(t)$; a convenient way of exhibiting the time-development of a function is

$$\begin{aligned} \frac{dg}{dt} &= \frac{\partial g}{\partial t} + \sum_k \left(\frac{\partial g}{\partial x_k} \frac{dx_k}{dt} + \frac{\partial g}{\partial p_k} \frac{dp_k}{dt} \right) \\ &= \frac{\partial g}{\partial t} + \sum_k \left(\frac{\partial g}{\partial x_k} \frac{\partial H}{\partial p_i} - \frac{\partial g}{\partial p_k} \frac{\partial H}{\partial x_i} \right) \\ &= \frac{\partial g}{\partial t} + [g, H] \end{aligned} \tag{G.10}$$

Note the similarity between this classical relation and Eqn. (12.88) for the time rate of change of expectation values of quantum operators.

Example G.1.

Using the Poisson bracket formalism, we can show that angular momentum is conserved for a central potential in three dimensions. The Hamiltonian function is given by

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(r) \tag{G.11}$$

where $r = \sqrt{x^2 + y^2 + z^2}$. We note that the force is given $\mathbf{F} = -\nabla V(r)$ so that

$$\frac{\partial V(r)}{\partial x} = (-F)\frac{x}{r} \tag{G.12}$$

and so forth.

(Continued)

Considering, for definiteness, the z component of angular momentum given by $L_z = xp_y - yp_x$, one can show that

$$\begin{aligned}\frac{dL_z}{dt} &= \frac{\partial L_z}{\partial t} + [L_z, H] \\ &= \left[\frac{\partial L_z}{\partial x}\frac{\partial H}{\partial p_x} - \frac{\partial L_z}{\partial p_x}\frac{\partial H}{\partial x}\right] + \left[\frac{\partial L_z}{\partial y}\frac{\partial H}{\partial p_y} - \frac{\partial L_z}{\partial p_y}\frac{\partial H}{\partial y}\right] + \left[\frac{\partial L_z}{\partial z}\frac{\partial H}{\partial p_z} - \frac{\partial L_z}{\partial p_z}\frac{\partial H}{\partial z}\right] \\ &= \left[(p_y)\left(\frac{p_x}{m}\right) - (-y)\left(-F\frac{x}{r}\right)\right] + \left[(-p_x)\left(\frac{p_y}{m}\right) - (x)\left(-F\frac{y}{r}\right)\right] \\ \frac{dL_z}{dt} &= 0 \end{aligned} \tag{G.13}$$

This relation also suggests that the Poisson bracket of two functions is the classical quantity which can be generalized in quantum mechanics to the commutator of two operators

$$[\hat{g}, \hat{h}] \equiv \hat{g}\hat{h} - \hat{h}\hat{g} \tag{G.14}$$

via

$$[g, h]_{\text{Poisson}} \longrightarrow [\hat{g}, \hat{h}] = i\hbar [g, h]_{\text{Poisson}} \tag{G.15}$$

The Hamiltonian for a charged particle acted on by electromagnetic fields is written in terms of the potentials, $\phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ via

$$H(\mathbf{r}, \mathbf{p}) = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{r}, t)\right)^2 + q\phi(\mathbf{r}, t) \tag{G.16}$$

To prove this requires one to show that the corresponding Hamilton's equations reproduce Newton's laws with the Lorentz force. The classical Hamiltonian in Eqn. (G.16) can be written more explicitly as

$$\begin{aligned} H = &\frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) - \frac{q}{m}\left(p_x A_x + p_y A_y + p_z A_z\right) \\ &+ \frac{q^2}{2m}\left(A_x^2 + A_y^2 + A_z^2\right) + q\phi \end{aligned} \tag{G.17}$$

Hamilton's equations for the x and p_x coordinates in this case become

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m} - \frac{q}{m}A_x \quad \text{or} \quad m\dot{x} = p_x - qA_x \tag{G.18}$$

and

$$
\begin{aligned}
-\dot{p}_x &= \frac{\partial H}{\partial x} \\
&= -\frac{q}{m}\left(p_x \frac{\partial A_x}{\partial x} + p_y \frac{\partial A_y}{\partial x} + p_z \frac{\partial A_z}{\partial x}\right) \\
&\quad + \frac{q^2}{2m}\left(A_x \frac{\partial A_x}{\partial x} + A_y \frac{\partial A_y}{\partial x} + A_z \frac{\partial A_x}{\partial x}\right) + q\frac{\partial \phi}{\partial x}
\end{aligned}
\tag{G.19}
$$

These can be combined by differentiating Eqn. (G.18) with respect to t provided one recalls that

$$
m\ddot{x} = \dot{p}_x - q\frac{dA_x}{dt} = \dot{p}_x - q\left(\frac{\partial A_x}{\partial t} + \dot{x}\frac{\partial A_x}{\partial x} + \dot{y}\frac{\partial A_x}{\partial y} + \dot{z}\frac{\partial A_x}{\partial z}\right) \tag{G.20}
$$

since $\mathbf{A} = \mathbf{A}(x(t), y(t), z(t); t)$ depends on time explicitly (through the t) and implicitly (through the time-dependent positions). The resulting equation for the x variable is then

$$
m\ddot{x} = q\left(\left\{-\frac{\partial \phi}{\partial x} - \frac{\partial A_x}{\partial t}\right\} + \left\{\dot{y}\left[\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right] + \dot{z}\left[\frac{\partial A_z}{\partial x} - \frac{\partial A_x}{\partial z}\right]\right\}\right) \tag{G.21}
$$

or

$$
m\ddot{x} = q\left(\mathbf{E}_x + (\mathbf{v} \times \mathbf{B})_x\right) \tag{G.22}
$$

since

$$
\mathbf{E} = -\nabla\phi(\mathbf{r}, r) - \frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}, t) \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r}, t) \tag{G.23}
$$

The Hamiltonian formalism also provides a way to describe classical probability distributions for position and momentum which can be compared to their quantum counterparts (as discussed in Sections 5.1 and 9.4). One starts with the notion of the *classical phase space*. For one particle in one dimension, this is the space of possible values of x and p, as in Fig. G1; for N particles in three dimensions, it is a $6N$-dimensional space corresponding to the possible values of $\mathbf{r}_i$, $\mathbf{p}_i$. Given a set of initial conditions, the solutions obtained from Newton's (or Hamilton's) equations for $x(t)$ and $p(t)$ trace out a trajectory in the phase space. For example, for a harmonic oscillator with initial conditions $x(0) = A$ and $\dot{x}(0) = 0$, the solutions are obviously

$$
x(t) = A\cos(\omega t) \quad \text{and} \quad p(t) = -\frac{A\omega}{m}\sin(\omega t) \tag{G.24}
$$

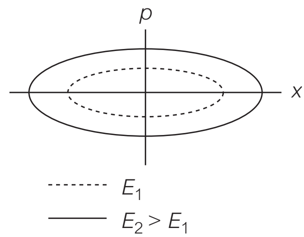

Figure G.1. Phase space diagram (plot of allowed values of p and x) for a single particle in a harmonic oscillator potential. The allowed "trajectories" in the parameter space in this case are determined by Eqn. (G.24).

which gives the elliptical path in phase space shown in Fig. G1. The form of this "trajectory" can be determined, even if we specify only the total energy, via the relation

$$E = H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{G.25}$$

The *phase space distribution*, $\rho(x, p)$, for a given value of E can then be written in the form

$$\rho(x, p) = K\delta(E - H(p, x)) \tag{G.26}$$

where the normalization constant is determined by the condition that

$$\int dx \int dp\ \rho(x, p) = 1 \tag{G.27}$$

The classical probability densities for position (x) or momentum (p) can be derived by integrating over the variable which is not specified; for example,

$$P_{\rm CL}(x) = \int dp\, \rho(x, p) \quad \text{and} \quad P_{\rm CL}(p) = \int dx\, \rho(x, p) \tag{G.28}$$

As an example, consider the Hamiltonian with a general potential energy function $V(x)$

$$H = \frac{p^2}{2m} + V(x) \tag{G.29}$$

If we write $p_0(x) = \sqrt{E - V(x)}$, the corresponding classical distribution in x will be given by

$$\begin{aligned} P_{\rm CL}(x) &= K \int dp\ \delta\left(E - \left(\frac{p^2}{2m} - V(x)\right)\right) \\ &\propto \int dp\ \delta\left(p^2 - 2m(E - V(x))\right) \\ &\equiv \int dp\ \delta\left(p^2 - p_0^2(x)\right) \end{aligned}$$

$$= \frac{1}{2|p_0(x)|} \int dp \left[\delta(p - p_0(x)) + \delta(p + p_0(x)\right]$$

$$\propto \frac{1}{\sqrt{E - V(x)}} \tag{G.30}$$

since $p_0^2(x) = 2m(E - V(x)$. This is the same result obtained in Sections 5.1 and 9.4.1, using more intuitive methods.

G.1 **Problems**

PG.1. Write down Hamilton's equations for the angular variable pair θ and $p_\theta = mr^2\theta$ where the Hamiltonian is

$$H = \frac{p_\theta^2}{2I} + V(\theta) \tag{G.31}$$

and show how the standard equations for rotational motion arise.

PG.2. Show that the Poisson bracket of the position and momentum coordinates of a multiparticle system satisfy

$$[x_i, x_j] = 0, \quad [p_i, p_j] = 0, \quad \text{and} \quad [x_i, p_j] = \delta_{i,j} \tag{G.32}$$

PG.3. Consider a harmonic oscillator for which the classical Hamiltonian is

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{G.33}$$

Use Eqn. (G.10) to show that the function

$$\phi(x, p_x; t) = i\left(\log(A) - \log(x - ip/m\omega)\right) - \omega t \tag{G.34}$$

is actually independent of time for this system. What is the physical significance of this variable?

PG.4. For the classical Kepler problem, defined by the Hamiltonian

$$H = \frac{1}{2m}\mathbf{p}^2 - \frac{k}{r} \tag{G.35}$$

show that the *Lenz–Runge vector* defined by

$$\mathbf{R} = \frac{\hat{\mathbf{r}}}{r} - \left(\frac{1}{mk}\right)\mathbf{p} \times \mathbf{L} \tag{G.36}$$

is a constant of the motion, that is it is conserved. Do this by showing that $d\mathbf{R}/dt = 0$ using the Poisson bracket formalism.

PG.5. Using the Hamiltonian corresponding to a linear confining potential

$$H = \frac{p^2}{2m} + C|x| \tag{G.37}$$

and Eqn. (G.28), derive $P_{\mathrm{CL}}(p)$.

PG.6. What does the classical phase space diagram look like for one particle in the one-dimensional infinite well, that is, what is the analog of Fig. G1? For the particle in the potential of PG.5? For an unbound free particle? For a particle subject to a constant force given by $V(x) = -Fx$? For a particle bouncing up and down on a table, with no energy loss, under the influence of gravity?