Chapter 11

Hamiltonian formulation

In reformulating mechanics in the language of a variational principle and Lagrangians in Chapter 4, we learned about a powerful new technology that helps us unravel dynamics more transparently and efficiently. Historically, this exercise in mathematical physics also inspired the development of quantum mechanics. Concurrent with this reformulation of mechanics, there is yet another picture of the same physics known as the *Hamiltonian formalism*, another of the outstanding contributions to mechanics made by the nineteenth-century Irish mathematician and physicist William Rowan Hamilton. Much like the Lagrangian approach, the Hamiltonian description of mechanics has given us a different perspective that is sometimes technically advantageous, and it has also played a crucial role in the emergence of quantum mechanics. In this chapter we develop the Hamiltonian formalism starting from the now-familiar Lagrangian approach. We explore examples that elucidate the advantages and disadvantages of this new approach, and develop the powerful related formalisms of canonical transformations, Poisson brackets, and Liouville's theorem.

11.1 Legendre transformations

We start with a preliminary mathematical construct known as the *Legendre transform*[1] to help us transition from the Lagrangian to the Hamiltonian for-

[1] Adrien-Marie Legendre (1752-1833) was a French mathematician and physicist who made a number of important contributions to applied mathematics and mathematical physics.

mulations of mechanics. The Legendre transform has many uses in physics: In addition to mechanics, it plays a particularly prominent role in thermodynamics and statistical mechanics. Let us then start with a general statement of the problem we wish to address.

Consider a function of two independent variables $A(x,y)$ - presumably of some physical importance - whose derivative

$$z = \frac{\partial A(x,y)}{\partial y} \tag{11.1}$$

is a measurable quantity that may be more interesting than y itself. For example, $A(x,y)$ may be a Lagrangian $L(q,\dot{q})$ and

$$p_k = \frac{\partial L}{\partial \dot{q}_k} \tag{11.2}$$

the momentum of a particle, a quantity that is conserved under certain circumstances, and therefore may be more interesting than the generalized velocity $\dot{q}_k$ we began with. We want to think of z as an independent variable and eliminate y in $A(x,y)$ in favor of z:

$$y \to z \ . \tag{11.3}$$

The reader may be tempted to accomplish this goal as follows: start with equation (11.1), and invert it to get $y(x,z)$; then substitute the result into $A(x,y(x,z)) \equiv B(x,z)$, thus eliminating y and retrieving a function of x and z alone. However, this naive approach throws away some of the information within $A(x,y)$! That is, unfortunately, $B(x,z)$ does *not* contain all the information in the original functional form of $A(x,y)$. To see this, consider an explicit example. Let

$$A(x,y) = x^2 + (y-a)^2 \tag{11.4}$$

where a is some constant. Then

$$z = \frac{\partial A}{\partial y} = 2\,(y-a) \Rightarrow y(x,z) = \frac{z}{2} + a \ . \tag{11.5}$$

Finally, eliminating y, we find that

$$A(x,y(x,z)) = x^2 + \frac{z^2}{4} \equiv B(x,z) \ . \tag{11.6}$$

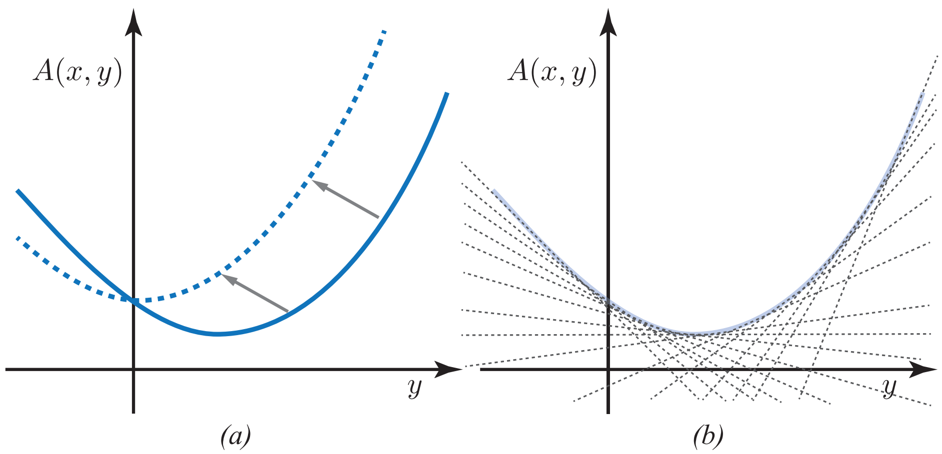

FIGURE 11.1 : (a) Two functions $A(x, y)$, differing by a shift, whose naive transformation through $y \to z$ lead to the same transformed function $B(x, z)$; (b) The envelope of $A(x, y)$ consisting of slopes *and* intercepts completely describe the shape of $A(x, y)$.

So we have eliminated y in favor of z, but we have lost the constant a! We would for example get the *same* $B(x, z)$ for two different functions $A(x, y)$ with different constants for a. Thus, the naive substitution $y \to z$ loses information present in the original function $A(x, y)$. If $A(x, y)$ were a Lagrangian, for example, we would lose part of the dynamics if we attempted to describe things with the transformed functional. We need instead a transformation that preserves *all* the information in the original function or functional.

The reason why the naive substitution does not work is simple. Our new independent variable $z = \partial A/\partial y$ is a *slope* of $A(x, y)$; and knowing the slope of a function everywhere does *not* determine the function itself: we can still shift the function around while maintaining the same slopes, as illustrated in Figure 11.1(a). To delineate the shape of $A(x, y)$, we need *both* its slopes and relevant intercepts of the straight lines that envelop $A(x, y)$, as depicted in Figure 11.1(b).

Let us denote the intercepts of such straight lines by $B(x, z)$, one for each slope[2] z. At every y there is a slope z, as well as a corresponding intercept $B(x, z)$. It is now easy to see that given $A(x, y)$ we can find $B(x, z)$, and vice versa: geometrically, we can see that given $A(x, y)$ we can determine the

[2]Note that if $A(x, y)$ is not monotonic in y, we may get a multiple-valued function in z for $B(x, z)$

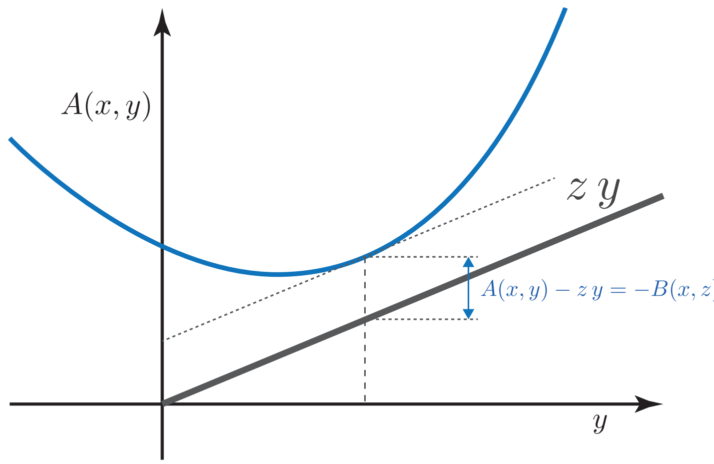

FIGURE 11.2 : The Legendre transformation of $A(x,y)$ as $B(x,z)$.

envelope of straight lines, and given the envelope of straight lines, we can reconstruct the shape of $A(x,y)$.

Algebraically, we can capture these statements by writing the negative of the intercept of each straight line in Figure 11.2 as

$$B(x,z) = z\,y - A(x,y) \tag{11.7}$$

where $y(x,z)$ is viewed as a function of x and z by using

$$z = \frac{\partial A(x,y)}{\partial y} \ . \tag{11.8}$$

to solve for $y(x,z)$. The vertical coordinate is $A(x,y)$, the slope is $z = \partial A/\partial y$, the horizontal coordinate is y, and the *negative* intercept is B. Therefore the equation of the straight line is $A(x,y) = z\,y + (-B(x,z))$. All the information in $A(x,y)$ can be found in a catalog of the slopes and intercepts of all the straight lines tangent to the curve $A(x,y)$.

This is the approach of Legendre to eliminating the variable y in favor of the new variable z. As argued above, $B(x,z)$ contains *all* the original information in the function $A(x,y)$. In short, instead of the naive substitution $A(x,y(x,z)) \to B(x,z)$ we started out with, we need to consider $z\,y(x,z) - A(x,y(x,z)) \to B(x,z)$. $B(x,z)$ is then known as the **Legendre transformation** of $A(x,y)$.

Let us summarize the process. We start with a given function $A(x, y)$ and then replace y with

$$z = \frac{\partial A(x, y)}{\partial y} \tag{11.9}$$

We invert the latter equation to get $y(x, z)$. Then we write the new Legendre transform of $A(x, y)$ as

$$B(x, z) = z\, y(x, z) - A(x, y(x, z)) \tag{11.10}$$

This process can be easily inverted. We note that

$$dB = zdy + ydz - \left(\frac{\partial A}{\partial x}\right) dx - \left(\frac{\partial A}{\partial y}\right) dy. \tag{11.11}$$

Using the chain rule, we can also write

$$dB = \left(\frac{\partial B}{\partial x}\right) dx + \left(\frac{\partial B}{\partial z}\right) dz, \tag{11.12}$$

so from (11.9), we get

$$y = \frac{\partial B}{\partial z} \tag{11.13}$$

and

$$-\frac{\partial A}{\partial x} = \frac{\partial B}{\partial x}. \tag{11.14}$$

Hence, the process of the inverse Legendre transform goes as follows. Given $B(x, z)$, the inverse Legendre transform replaces z back with y by starting from

$$y = \frac{\partial B}{\partial z}\ , \tag{11.15}$$

inverting it to get $z(x, y)$, and substituting in

$$A(x, y) = z(x, y)\, y - B(x, z(x, y)) \tag{11.16}$$

to retrieve $A(x, y)$. All along, we also have the relation between the derivative of passive variables given by (11.14). The variables y and z are called the **active variables**, while x is called the **passive** or **spectator** variable of the transform.

EXAMPLE 11-1: A simple Legendre transform

Let us compute properly the Legendre transform of the function we already encountered,

$$A(x,y) = x^2 + (y-a)^2 \ . \tag{11.17}$$

Start with the derivative, which is to become our new independent variable,

$$z = \frac{\partial A(x,y)}{\partial y} = 2\,(y-a) \ . \tag{11.18}$$

Solving for y,

$$y(x,z) = \frac{z}{2} + a \ . \tag{11.19}$$

The Legendre transform of $A(x,y)$ is then

$$\begin{aligned} B(x,z) &= z\,y(x,z) - A(x,y(x,z)) = z\left(\frac{z}{2}+a\right) - \left(x^2 + \frac{z^2}{4}\right) \\ &= \frac{1}{4}\,(z+2\,a)^2 - x^2 - a^2 \ , \end{aligned} \tag{11.20}$$

demonstrating that we have now kept track of the original a dependence in the transform $B(x,z)$. We can also verify equation (11.14),

$$\frac{\partial B}{\partial x} = -2\,x = -\frac{\partial A}{\partial x} \ . \tag{11.21}$$

11.2 Hamilton's equations

We now proceed to apply a Legendre transform specifically to the Lagrangian. The object of interest is not a function, but a functional

$$L(q(t), \dot{q}(t), t) \tag{11.22}$$

of N degrees of freedom $q_k(t)$. The variational principle yields N second-order differential equations for N degrees of freedom. This requires $2\,N$ initial constants to predict the trajectory of the system. For example, we may specify

$$\{q_k(0), \dot{q}_k(0)\} \ . \tag{11.23}$$

Our proposal is to rewrite the dynamics in terms of $2\,N$ *first* order differential equations, which, as required, would still require $2\,N$ initial conditions – one for each of the first order differential equations. *In short, the aim is to reduce the order of the differential equations by one at the expense of doubling the number of independent equations.*

To reduce the order of the differential equations of motion, we need to eliminate $\dot{q}_k$: after all, the second derivative $\ddot{q}_k$ in the equations of motion arises generically from the time derivative of the $\partial L/\partial \dot{q}_k$ term in Lagrange's equations. Since the dynamics is packaged within the Lagrangian, we also need to preserve all the information in L in this process. Hence, we apply a Legendre transformation with the active variables

$$\dot{q}_k \to p_k = \frac{\partial L}{\partial \dot{q}_k} \tag{11.24}$$

using equation (11.9)). The canonical momenta p_k are the new independent variables that are to replace the $\dot{q}_k$'s. The passive variables are $q_k(t)$ and t. Using (11.24, we invert and obtain $\dot{q}_k(t,q,p)$ and substitute in

$$p_k\dot{q}_k - L(q,\dot{q},t) \equiv H(q,p,t) \tag{11.25}$$

using equation (11.10) for each of the N $\dot{q}_k$'s. The quantity $H(q,p,t)$ is then the Legendre transform of the Lagrangian – actually it involves N Legendre transforms. Interestingly, H is what we called earlier in the text the **Hamiltonian**! That is, we have already encountered the Legendre transform of the Lagrangian: it is the extremely useful quantity we have already named the Hamiltonian, which in many situations (but not all) is simply the energy of the particle.

Where are the promised first-order differential equations? We know from the inverse Legendre transform relation that (using equation (11.13))

$$\dot{q}_k = \frac{\partial H}{\partial p_k}\ . \tag{11.26}$$

These are only N first order differential equations for the $2\,N$ independent variables q_k and p_k. Note, however, that the passive variable derivative relations of equation (11.14)are

$$-\left(\frac{\partial L}{\partial q_k}\right) = \frac{\partial H}{\partial q_k} \tag{11.27}$$

and

$$-\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \ . \tag{11.28}$$

Using the Lagrange equations of motion, we can then write

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_k}\right) = \dot{p}_k = \frac{\partial L}{\partial q_k} = -\frac{\partial H}{\partial q_k} \ , \tag{11.29}$$

or, more directly,

$$\dot{p}_k = -\frac{\partial H}{\partial q_k} \ . \tag{11.30}$$

These are an additional set of N first order differential equations. Along with equations (11.26), they constitute a set of $2N$ first order differential equations for $2N$ independent variables $q_k(t)$ and $p_k(t)$.

Finally, using the chain rule and equations (11.26)) and (11.30, we get

$$\frac{\partial H}{\partial t} = \frac{dH}{dt} - \frac{\partial H}{\partial q_k}\dot{q}_k - \frac{\partial H}{\partial p_k}\dot{p}_k = \frac{dH}{dt} \tag{11.31}$$

which, given (11.28), implies

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} \ . \tag{11.32}$$

The latter should look familiar: when the Lagrangian does not depend on time, the Hamiltonian is conserved!

Let us end by summarizing this interesting transformation from second to first order differential equations. Given a Lagrangian with N degrees of freedom, we transform it to a Hamiltonian

$$L(q_k, \dot{q}_k, t) \to H(q_k, p_k, t) \tag{11.33}$$

with $2N$ independent degrees of freedom: the q_k's and the p_k's. To do this, we write

$$p_k = \frac{\partial L}{\partial \dot{q}_k}, \tag{11.34}$$

which gives us the functions $p_k(q, \dot{q}, t)$. We invert these functions to get $\dot{q}_k(q, p, t)$ and and substitute in

$$H(q, p, t) = p_k \dot{q}_k - L \ . \tag{11.35}$$

The dynamics is now tracked by the variables $q_k(t)$ and $p_k(t)$. This $2N$ dimensional space is called **phase space**. The time evolution is described in phase space through $2N$ *first* order differential equations

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \quad , \quad \dot{p}_k = -\frac{\partial H}{\partial q_k} \tag{11.36}$$

together with

$$\frac{\partial L}{\partial t} = -\frac{dH}{dt} \tag{11.37}$$

implying that a time-independent Lagrangian yields a conserved Hamiltonian. Equations (11.36) are **Hamilton's equations of motion.** They consist of twice as many equations as the Lagrange equations, but they are always first order rather than second order, and therefore have certain advantages.

Let us emphasize once again that in order to use Hamilton's equations, it is essential to write the Hamiltonian function in terms of the generalized coordinates q_k and their canonical momenta p_k! *There must be no generalized velocities $\dot{q}_k$ remaining in H!* [3] So again, the steps are:

1. Write down the Lagrangian $L = L(q_k, \dot{q}_k.t)$ of the system
2. Find the canonical momenta $p_k = \partial L/\partial \dot{q}_k$
3. Find the Hamiltonian $H = \sum_i p_i \dot{q}_i - L(q_k, \dot{q}_k, t)$
4. Eliminate all the $\dot{q}_k$ in H in favor of the $p's$ and $q's$, giving $H(q_k, p_k, t)$
5. Write out Hamilton's equations of motion, a set of 2N first-order differential equations.

In terms of analytic problem-solving, Hamilton's equations add to our arsenal of techniques. However, the real advantages of Hamilton's equations are not primarily in analytic problem-solving, but in the following. (i) They give insight into understanding motion, particularly in phase space: The Hamiltonian framework gives us a qualitative bird's-eye perspective of dynamics

[3] It is a common error to write the Hamiltonian by its definition $H = \sum_i p_i \dot{q}_i - L(q_k, \dot{q}_k, t)$ and forget to eliminate the $\dot{q}_k$ in favor of the p_k and q_k before using Hamilton's equation $\dot{p}_k = \partial H/\partial q_k$. Doing this will give an incorrect equation of motion!

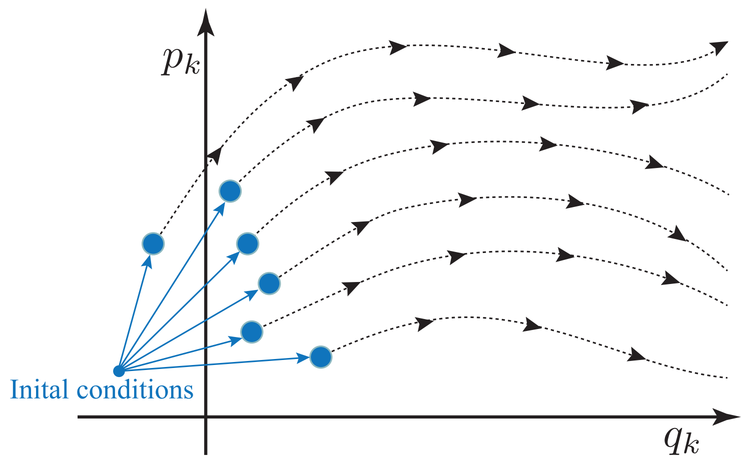

FIGURE 11.3 : The two dimensional cross section of a phase space for a system. The flow lines depict Hamiltonian time evolution.

without solving any differential equations at all. (ii) They are more immediately appropriate for numerical solutions, a very important advantage, since relatively few problems in mechanics can be solved exactly in terms of established functions. That is, they are more easily implemented in computer algorithms than second-order differential equations, resulting in more stable numerical solutions of complex systems. (iii) They provide a natural bridge from classical to quantum mechanics, a bridge that was exploited in very different ways by two originators of quantum mechanics, the Austrian-born physicist Erwin Schŕodinger (1887-1961) and the German physicist Werner Heisenberg (1901-1976).

11.3 Phase Space

Figure 11.3 depicts a two-dimensional cross section of a phase space. A point in phase space is a complete description of the system at an instant in time. Any such point may be viewed as a complete specification of the initial conditions at time zero, and we evolve from this point along the $2N$ dimensional vector field

$$\{\dot{q}_1, \dot{p}_1, \dot{q}_2, \dot{p}_2, \cdots, \dot{q}_N, \dot{p}_N\} = \left\{\frac{\partial H}{\partial p_1}, -\frac{\partial H}{\partial q_1}, \frac{\partial H}{\partial p_2}, -\frac{\partial H}{\partial q_2}, \cdots, \frac{\partial H}{\partial p_N}, -\frac{\partial H}{\partial q_N}\right\} \quad (11.38)$$

as shown in the figure. The initial state of the system then traces a smooth line in phase space as it evolves into the future. Notice that this evolution is *almost* a gradient flow – that is a flow along the gradient of a function. It is so *except* for a minus sign in half of the terms of (11.38). This additional "twist" lies at the heart of dynamics. We will revisit it at the end of this part of the book, along with the insight it gives us into quantum mechanics.

EXAMPLE 11-2: The simple harmonic oscillator

Consider a particle of mass m moving in one dimension under the influence of a spring with force constant k. The Lagrangian is

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2 \; . \tag{11.39}$$

We have $N = 1$ degree of freedom, and so the corresponding phase space is $2N = 2$ dimensional. Let us parametrize it by $\{x, p\}$, where

$$p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}. \tag{11.40}$$

We now invert this relation in preparation for writing the Hamiltonian, giving

$$\dot{x} = \frac{p}{m} \tag{11.41}$$

This allows us to eliminate $\dot{x}$,

$$H(x,p) = \dot{x}p - L = \frac{p^2}{m} - \left(\frac{p^2}{2\,m} - \frac{1}{2}kx^2\right) = \frac{p^2}{2\,m} + \frac{1}{2}kx^2 \tag{11.42}$$

which gives us the Legendre transform of the original Lagrangian, the Hamiltonian, which is also the energy in this case. *Note that the generalized velocity $\dot{x}$ is (correctly) absent from the Hamiltonian.* The equations of motion are now first order,

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \quad , \quad \dot{p} = -\frac{\partial H}{\partial x} = -kx \; . \tag{11.43}$$

While rather depressingly simple, we can now implement this dynamics on a computer. More interestingly, we can now visualize the evolution in an interesting way, as shown in Figure 11.4. From (11.37), we know the Hamiltonian is conserved

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t} = 0 \; . \tag{11.44}$$

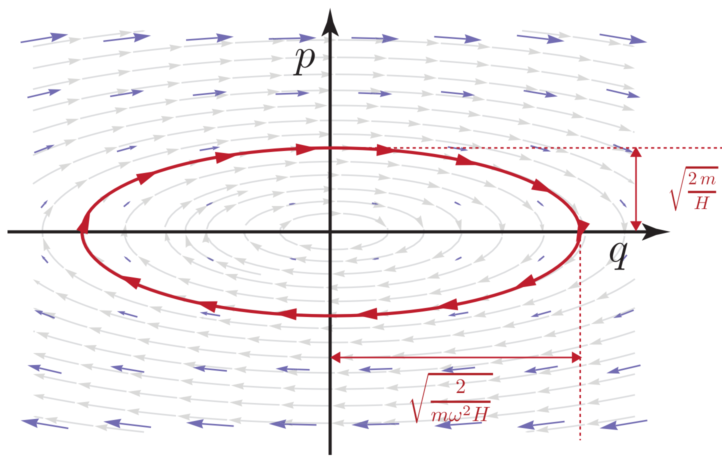

FIGURE 11.4 : The phase space of the one dimensional simple harmonic oscillator.

Hence, the trajectories in phase space are contours of constant H. From (11.42), we see that these are ellipses with semimajor and semiminor axes as shown in the figure. Note also the direction of flow in phase space: pick any point on an ellipse as your initial condition, and from the sign of p deduce the direction of flow as shown. An interesting aspect of this picture is that we are able to get a quick birds-eye view of the dynamics in the space of all initial conditions. In this simple example, there are no interesting regions of the phase space that result in qualitatively different evolutionary patterns. However, in more complex system, a quick stare at the phase space can immediately identify interesting basins of initial conditions, as we shall see. Nevertheless, the phase-space picture already constitutes a quick proof that all time developments of the simple harmonic oscillator are necessarily *closed* and *bounded*. This means we expect that there is a period after which the time evolution repeats itself; and that the particle can never fly off to infinity. These statements are non-trivial, particularly for more complex systems. Note also that drawing the phase space does not involve solving any differential equations: it is simply the task of drawing contours of the algebraic expression given by H.

Now what if we want to solve our first-order differential equations (11.43) *analytically*? While their first-order nature is welcome, the two equations are in fact coupled. To decouple them, we unfortunately need to hit the first equation of (11.43) with a time derivative

$$\ddot{x} = \frac{\dot{p}}{m} = -\frac{k}{m}x, \tag{11.45}$$

bringing us back to the second-order differential equation that is the simple harmonic oscillator equation. In this case, the Hamiltonian picture did not help us solve the time evolution beyond what the Lagrangian formalism can do more easily: From that perspective it seems like a waste of time! But even in this simple case, we learned about the geometry of the space of initial conditions through phase space; and as we shall see, we developed a framework particularly suited for a numerical, computer-based solution of the dynamics.

As the systems of interest get more and more complicated, we will see more and more benefits from analyzing it with the Hamiltonian formalism. We can think of the Hamiltonian picture as one of several different ways of looking at a system, each having advantages and disadvantages; and together, these methods make up a powerful arsenal of tools that help us understand complex dynamics. ———————————————————————

EXAMPLE 11-3: A bead on a parabolic wire

Consider a bead of mass m constrained to move along a vertically-oriented parabolic wire in the presence of a uniform gravitational field g. We write the Lagrangian as

$$L = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2\right) - mgy \tag{11.46}$$

with the constraint

$$y = \frac{x^2}{2} \ , \tag{11.47}$$

which is the shape of the wire. Implementing the constraint, we get a Lagrangian with a single degree of freedom,

$$L = \frac{m}{2}\left(1 + x^2\right)\dot{x}^2 - \frac{mg}{2}x^2 \ . \tag{11.48}$$

We expect a two-dimensional phase space, say parameterized by $\{x, p_x\}$, where

$$p_x = \frac{\partial L}{\partial \dot{x}} = m\left(1 + x^2\right)\dot{x} \Rightarrow \dot{x} = \frac{p_x}{m\left(1 + x^2\right)} \tag{11.49}$$

We then can write the Hamiltonian in terms of x and p_x by eliminating $\dot{x}$,

$$H = p_x\dot{x} - L = \frac{p_x^2}{2m\left(1 + x^2\right)} + \frac{mg}{2}x^2 \ . \tag{11.50}$$

Once again, since $\partial L/\partial t = 0$, the Hamiltonian is conserved, as implied by equation (11.37). Thus trajectories in phase space follow contours of constant H. Figure 11.5 shows a plot of the contours of H in phase space. We see a much richer structure of initial conditions than the case of the simple harmonic oscillator of the previous example. In particular, we see the stable point at $x = p_x = 0$. And we note that the system spends a great deal of time at the turning points $x_{\min}$ and $x_{\max}$. Indeed, we can easily perform statistics on the figure to determine the fraction of time the particle is near the turning points, find the maximum and even minimum momentum, and determine various qualitative and quantitative aspects of the

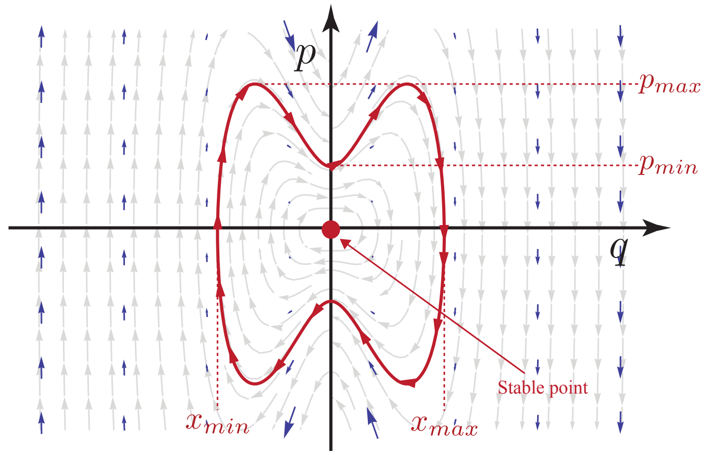

FIGURE 11.5 : The phase space of the one dimensional particle on a parabola problem.

dynamics - all without solving the equations of motion. We also note, as expected intuitively, that the orbits are all bounded and closed.

The two first order equations of motion are given by (equations (11.36))

$$\dot{x} = \frac{p_x}{m\left(1+x^2\right)} \tag{11.51}$$

$$\dot{p}_x = -mgx + \frac{x p_x^2}{m\left(1+x^2\right)^2} \ . \tag{11.52}$$

Once again, these are coupled first-order differential equations. Attempting to decouple them leads generically to second order equations, the Lagrangian equations of motion. However, it is particularly easy to code these first-order differential equations into a computer algorithm.

EXAMPLE 11-4: A charged particle in a uniform magnetic field

A particle of mass m and charge q moves around in three dimensions in the background of given electric and magnetic fields. The Lagrangian was developed in Chapter 8 and is given by

$$L = \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) - q\phi + \frac{q}{c}\dot{x}A_x + \frac{q}{c}\dot{y}A_y + \frac{q}{c}\dot{z}A_z \tag{11.53}$$

where $\phi(x, y, z, t)$ and $\boldsymbol{A}(x, y, z, t)$ are respectively the electric potential and the vector potential. To transform to the Hamiltonian picture, we write the canonical momenta (equation (11.34))

$$\begin{aligned} p_x &= \frac{\partial L}{\partial \dot{x}} = m\dot{x} + \frac{q}{c}A_x \\ p_y &= \frac{\partial L}{\partial \dot{y}} = m\dot{y} + \frac{q}{c}A_y \\ p_z &= \frac{\partial L}{\partial \dot{z}} = m\dot{z} + \frac{q}{c}A_z \end{aligned} \tag{11.54}$$

or more compactly

$$\boldsymbol{p} = m\boldsymbol{v} + \frac{q}{c}\boldsymbol{A} \Rightarrow \boldsymbol{v} = \frac{\boldsymbol{p}}{m} - \frac{q}{mc}\boldsymbol{A} \tag{11.55}$$

where in the last step, we solved for $\boldsymbol{v}$ in preparation for eliminating the $\boldsymbol{v}$ dependence in the Hamiltonian (equation (11.35))

$$H = \boldsymbol{v} \cdot \boldsymbol{p} - L = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\phi \tag{11.56}$$

In the Hamiltonian picture, the effect of the electromagnetic fields is then simply the shifting of the momenta $\boldsymbol{p} \to \boldsymbol{p} - (q/c)\boldsymbol{A}$ and the addition of the electric potential energy $q\phi$.

As we saw in Chapter 8, the magnetic field is given in terms of the vector potential by $\boldsymbol{B} = \nabla \times \boldsymbol{A}$, for a uniform magnetic field in the z direction, $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$, we can write a vector potential

$$\boldsymbol{A} = -\frac{1}{2}B_0 y\,\hat{\boldsymbol{x}} + \frac{1}{2}B_0 x\,\hat{\boldsymbol{y}} \tag{11.57}$$

which is given in the Coulomb gauge choice. Substituting this intoequation (11.56) and noting that the Hamiltonian is conserved since $\partial L/\partial t = 0$, we have

$$H = \frac{1}{2\,m}\left(p_x - \frac{q\,y\,B_0}{2\,c}\right)^2 + \frac{1}{2\,m}\left(p_y + \frac{q\,x\,B_0}{2\,c}\right)^2 + \frac{1}{2\,m}p_z^2 \tag{11.58}$$

describing the constant Hamiltonian contours in phase space. As expected, the dynamics in the z direction is that of a free particle. In the x-y plane, we know the particle would be circling around. In phase space, if we focus say on the x-p_x cross section, we have off-center ellipses as show in Figure 11.6: In the (x, p_x) coordinates, the center is located at $(-2\,c\,p_y/q\,B_0, q\,y\,B_0/2\,c)$, and the radii are $(\sqrt{8\,m\,c^2 H/q^2 B_0^2}, \sqrt{2\,m\,H})$. More interestingly, in the x-y plane, we have shifted *circles* of radius

$$R = \sqrt{\frac{8\,m\,c^2}{q^2 B_0^2}\left(H - \frac{p_z^2}{2\,m}\right)}\,. \tag{11.59}$$

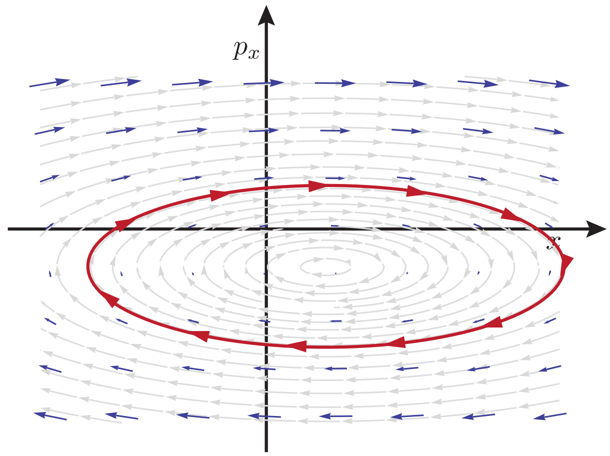

FIGURE 11.6 : The flow lines in the x-p_x cross section of phase space for a charged particle in a uniform magnetic field.

11.4 Canonical transformations

From the perspective of the Hamiltonian formalism, the playground for dynamics becomes phase space. Figure 11.7(a) shows a two dimensional cross section of a phase space. The flow lines depict the time evolution of the system with various initial conditions. Based on our experience, we know that coordinate transformations can be very useful when tackling physics problems. What if we were to apply a coordinate transformation directly in phase space

$$q_k \to Q_k(q,p,t) \quad , \quad p_k \to P_k(q,p,t) \ ? \tag{11.60}$$

To specify the full coordinate transformation in phase space, it then seems we would need $2N$ functions. Such a general coordinate transformation would also deform and distort the time evolution flow pattern as illustrated in Figure 11.7(b). However, in general, the new flow lines may not be *Hamiltonian*: by that we mean that the elegant attribute of time evolution in phase space as one given by the twisted gradients (*i.e.*, equation (11.38)) of a function called the Hamiltonian may not persist in $\{Q, P\}$ space

$$\dot{Q} \neq \frac{\partial f}{\partial P} \quad , \quad \dot{P} \neq -\frac{\partial f}{\partial Q} \tag{11.61}$$

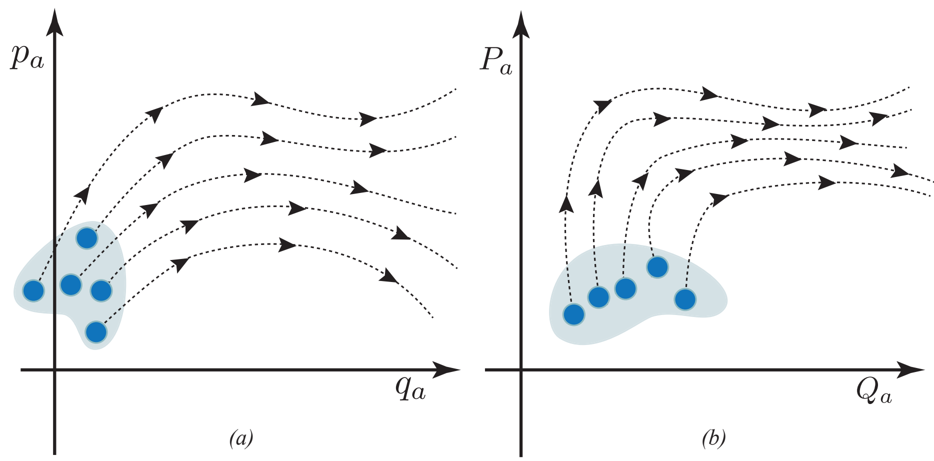

FIGURE 11.7 : (a) The flow lines in a given phase space; (b) The same flow lines as described by transformation coordinates and momenta.

for any *arbitrary* function $f(Q, P)$. The more interesting transformations in phase space are obviously those that preserve this interesting structure of Hamiltonian dynamics. We hence look for a subset of all possible transformations that preserve Hamiltonian structure; that is, through the transformation we obtain a new Hamiltonian

$$H(q,p) \to \widetilde{H}(Q,P) \tag{11.62}$$

such that

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \quad , \quad \dot{p}_k = -\frac{\partial H}{\partial q_k} \tag{11.63}$$

implies

$$\dot{Q}_k = \frac{\partial \widetilde{H}}{\partial P_k} \quad , \quad \dot{P}_k = -\frac{\partial \widetilde{H}}{\partial Q_k} \tag{11.64}$$

This is a non-trivial condition on the allowed transformations. We henceforth refer to such transformations as **canonical transformations**.

Let us find the general attributes of such canonical transformations. The structure of the Hamiltonian equations (11.63)) and (11.64 descends from the variational principle: the equations of motion are at the extremum of a single functional called the action. If the structure is to be preserved by a canonical transformation of phase space, and the equations of motion in the old and new variables are to be describing the same physical situation, we must require that the actions in the old and new coordinates remain unchanged,

$$S[q, \dot{q}, t] = S[Q, \dot{Q}, t] \ . \tag{11.65}$$

Since the action is the time integral of the Lagrangian, this implies that

$$L(q, \dot{q}, t) = \widetilde{L}(Q, \dot{Q}, t) + \frac{dF}{dt} \tag{11.66}$$

where the difference between the two Lagrangian can be a total time derivative dF/dt of an arbitrary function that vanishes at early and late times, since

$$\int_{t_0}^{t_1} dt\, \frac{dF}{dt} = F(t_1) - F(t_0) = 0 \ , \tag{11.67}$$

i.e., the time integral of the latter would then be inconsequential to the equations of motion. Using the Legendre transform between a Lagrangian and its Hamiltonian, we can then write

$$\dot{q}_k p_k - H = \dot{Q}_k P_k - \widetilde{H} + \frac{dF(q, p, Q, P, t)}{dt}. \tag{11.68}$$

The chain rule of multivariable calculus tells us that

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q_k}\dot{q}_k + \frac{\partial F}{\partial p_k}\dot{p}_k + \frac{\partial F}{\partial Q_k}\dot{Q}_k + \frac{\partial F}{\partial P_k}\dot{P}_k \ . \tag{11.69}$$

Substituting this into (11.68) we see that one way of satisfying this condition is

$$F \to F_1(q, Q, t) \tag{11.70}$$

with

$$p_k = \frac{\partial F_1(q, Q, t)}{\partial q_k} \qquad P_k = -\frac{\partial F_1(q, Q, t)}{\partial Q_k} \quad \text{and} \quad H = \widetilde{H} - \frac{\partial F_1}{\partial t} \tag{11.71}$$

To obtain the desired transformations $Q_k(q, p, t)$ and $P_k(q, p, t)$, we invert the first equation to get $Q_k(q, p, t)$; and we use this in the second equation to get $P_k(q, p, t)$. Finally, we use the third equation to solve for the desired new Hamiltonian $\widetilde{H}$. We have hence found that we can generate a canonical transformation from $\{q_k, p_k\}$ to $\{Q_k, P_k\}$ using a function $F_1(q, Q, t)$ and its derivatives. The function $F_1(q, Q, t)$ is called the **generator** of the canonical transformation.

EXAMPLE 11-5: Transforming the simple harmonic oscillator

Consider once again the celebrated simple harmonic oscillator: a particle of mass m in one dimension connected to a spring with the Hamiltonain

$$H = \frac{p^2}{2\,m} + \frac{1}{2} m\omega^2 q^2 \tag{11.72}$$

where $\omega = \sqrt{k/m}$ is the natural frequency, with k being the spring constant. The phase space is two dimensional, parameterized by $\{q, p\}$. Let us apply the canonical transformation using the generator

$$F_1(q, Q, t) = q\,Q. \tag{11.73}$$

From (11.71), we immediately get

$$p = Q \qquad P = -q \tag{11.74}$$

which can be inverted to give $Q(q, p) = p$ and $P(q, p) = -q$. The transformation exchanges position and momenta – along with the ubiquitous minus sign that is the hallmark of Hamiltonian dynamics! The new Hamiltonian is then

$$\widetilde{H} = \frac{p^2}{2\,m} + \frac{1}{2} m\omega^2 q^2 + 0 = \frac{Q^2}{2\,m} + \frac{1}{2} m\omega^2 P^2, \tag{11.75}$$

and the new equations of motion are

$$\dot{Q} = \frac{\partial \widetilde{H}}{\partial P} = m\omega^2 P \qquad \dot{P} = -\frac{\partial \widetilde{H}}{\partial Q} = -\frac{Q}{m} \tag{11.76}$$

This $\{Q, P\}$ system is physically equivalent to the $\{q, p\}$ system. We may say that, as far as dynamics is concerned, coordinates and momenta can be mixed and even exchanged; they must be different facets of the same physical information, somewhat like the mixing of energy and momentum when changing inertial perspectives in relativistic dynamics!

How about a canonical transformation that is simply the identity transformation

$$p_k = P_k \qquad q_k = Q_k \tag{11.77}$$

Using (11.71), we get

$$p_k = \frac{\partial F_1}{\partial q_k} = P_k \Rightarrow F_1 = P_k q_k + f(Q) \tag{11.78}$$

and

$$P_k = -\frac{\partial F_1}{\partial Q_k} = -\frac{\partial f}{\partial Q_k} \Rightarrow f(Q) = Q_k P_k \;!? \tag{11.79}$$

This is a contradiction, since our starting point assumption was that F_1 is a function of q_k, Q_k, and t only. Hence, it seems that $F_1(q, Q, t)$ cannot generate the identity transformation! Obviously, the identity transformation is canonical, hence we must have missed something in going from (11.68)) and (11.69) to (11.70.

Let us go back to equations (11.68)) and (11.69. $F_1(q, Q, t)$ is not the only class for generators that can solve these equations. Start by writing

$$\dot{Q}_k P_k = -Q_k \dot{P}_k + \frac{d}{dt}\left(Q_k P_k\right) \tag{11.80}$$

using the product rule. Substituting this in (11.68), we get

$$\dot{q}_k p_k - H = -Q_k \dot{P}_k - \widetilde{H} + \frac{d}{dt}\left(Q_k P_k + F_1\right) \tag{11.81}$$

Writing

$$F_2 = F_1(q, Q, t) + Q_k P_k, \tag{11.82}$$

we can now see that a generator of the form $F_2(q, P, t)$ has the correct structure to satisfy (11.81) if

$$p_k = \frac{\partial F_2}{\partial q_k} \qquad Q_k = \frac{\partial F_2}{\partial P_k} \tag{11.83}$$

and

$$H = \widetilde{H} - \frac{\partial F_2}{\partial t}\;. \tag{11.84}$$

Looking back at (11.82)), (11.83), and (11.84, and these set of equations, we notice that $F_2(q, P, t)$ is simply that Legendre transform of $F_1(q, Q, t)$

which replaces the Q_k's with P_k's! However, unlike $F_1(q, Q, t)$, the function $F_2(q, P, t)$ *does* include the identity transformation. Consider

$$F_2(q, P, t) = q_k P_k \tag{11.85}$$

where k is summed over. Using (11.83), we get

$$p_k = P_k \qquad Q_k = q_k \tag{11.86}$$

which is the sought for identity transformation.

This treatment also makes it clear that we can have two more classes of generators of canonical transformations: $F_3(p, Q, t)$ obtained through a Legendre transform of $F_1(q, Q, t)$ by replacing q_k's with p_k's; and $F_4(p, P, t)$ through a double Legendre transform by replacing q_k's with p_k's *and* replacing Q_k's with P_k's. To find $F_3(p, Q, t)$, start by writing

$$\dot{q}_k p_k = -q_k \dot{p}_k + \frac{d}{dt}\left(q_k p_k\right) \tag{11.87}$$

and substitute in (11.68). We then need

$$F \to F_3(p, Q, t) \tag{11.88}$$

with

$$q_k = -\frac{\partial F_1}{\partial p_k} \qquad P_k = -\frac{\partial F_1}{\partial Q_k} \tag{11.89}$$

and

$$H = \widetilde{H} - \frac{\partial F_3}{\partial t}\ . \tag{11.90}$$

To find $F_4(p, P, t)$ use both (11.80)) and (11.87) in (11.68. We then need

$$F \to F_4(p, P, t) \tag{11.91}$$

with

$$q_k = -\frac{\partial F_1}{\partial p_k} \qquad Q_k = \frac{\partial F_1}{\partial P_k} \tag{11.92}$$

and

$$H = \widetilde{H} - \frac{\partial F_4}{\partial t}\ . \tag{11.93}$$

This concludes the list of all possible canonical transformations. They are described by four classes of generators $F_1(q,Q,t)$, $F_2(q,P,t)$, $F_3(p,Q,t)$, and $F_4(p,P,t)$. To summarize, the transformations are extracted from these generators through

$$\begin{array}{lll} \text{For } F_1(q,Q,t): & p_k = \partial F_1/\partial q_k & P_k = -\partial F_1/\partial Q_k \\ \text{For } F_2(q,P,t): & p_k = \partial F_2/\partial q_k & Q_k = \partial F_2/\partial P_k \\ \text{For } F_3(p,Q,t): & q_k = -\partial F_3/\partial p_k & P_k = -\partial F_3/\partial Q_k \\ \text{For } F_4(p,P,t): & q_k = -\partial F_4/\partial p_k & Q_k = \partial F_4/\partial P_k \end{array} \tag{11.94}$$

And we always have

$$H = \widetilde{H} - \frac{\partial F}{\partial t} \tag{11.95}$$

Notice the pattern in these equations: coordinate and momenta are paired in each statement, *i.e.*, p_k with q_k and P_k with Q_k in $F_1(q,Q,t)$; and the rest are obtained by exchanging within these pairs – along with a flip of a sign for every exchange. $F_1(q,Q,t)$, $F_2(q,P,t)$, $F_3(p,Q,t)$, and $F_4(p,P,t)$ are related to each other by Legendre transformations

$$\begin{aligned} F_2(q,P,t) &= F_1(q,Q,t) + Q_k P_k \\ F_3(p,Q,t) &= F_1(q,Q,t) - q_k p_k \\ F_4(p,P,t) &= F_1(q,Q,t) + P_k Q_k - q_k p_k \end{aligned} \tag{11.96}$$

EXAMPLE 11-6: Identities

A particularly simply class of canonical transformations are the so-called "identities". One can easily check the following base transformations:

$$\text{For } F_1(q,Q,t) = q_k Q_k \Rightarrow \quad p_k = Q_k \qquad P_k = -q_k \tag{11.97}$$

$$\text{For } F_2(q,P,t) = q_k P_k \Rightarrow \quad p_k = P_k \qquad Q_k = q_k \tag{11.98}$$

$$\text{For } F_3(p,Q,t) = p_k Q_k \Rightarrow \quad q_k = -Q_k \qquad P_k = -p_k \tag{11.99}$$

$$\text{For } F_4(p,P,t) = p_k P_k \Rightarrow \quad q_k = -P_k \qquad Q_k = p_k \tag{11.100}$$

We see that the simplest non-trivial transformation for $F_1(q,Q,t)$ is the exchange of coordinates and momenta (with a minus sign twist); for $F_2(q,P,t)$, it is the usual identity transformation; for $F_3(p,Q,t)$, it is a reflection of both coordinates and momenta; and finally for $F_4(p,P,t)$, it is again an exchange of coordinates and momenta.

EXAMPLE 11-7: Infinitesimal transformations and the Hamiltonian

Infinitesimal transformations - those that are *almost* the identity - are often useful in physics as the building blocks of larger transformations. Let us consider the class of infinitesimal canonical transformations

$$F_2 = q_k P_k + \epsilon G(q,P,t) \tag{11.101}$$

where ϵ is taken as small, and $G(q,P,t)$ is an unknown function. From (11.94), we get

$$p_k = P_k + \epsilon \frac{\partial G}{\partial q_k} \qquad Q_k = q_k + \epsilon \frac{\partial G}{\partial P_k} \tag{11.102}$$

These transformations may look eeringly familiar... to see this, let us pretend we chose $G(q,P,t)$ such that $P_k = p_k(t+\delta t)$ and $Q_k = q_k(t+\delta t)$ and $\epsilon = \delta t$. That is, we transform the q_k's and p_k's to their values a small instant in time later. We then get

$$\dot{P}_k = -\frac{\partial G(q,P,t)}{\partial q_k} \qquad \dot{q}_k = \frac{\partial G(q,P,t)}{\partial P_k} \tag{11.103}$$

Since the Q_k's and P_k's differ from the q_k's and p_k's by an amount of the order of ϵ, to linear order in ϵ we can write these equations as

$$\dot{p}_k = -\frac{\partial G(q,p,t)}{\partial q_k} \qquad \dot{q}_k = \frac{\partial G(q,p,t)}{\partial p_k}. \tag{11.104}$$

If we then identify

$$H(q,p,t) \to G(q,P,t) \tag{11.105}$$

we notice that these are simply the Hamilton equations of motion! Put differently, Hamiltonian evolution is a canonical transformation with the infinitesimal generator of the transformation being the Hamiltonian! We can then view time evolution as a canonical transformation to coordinates an instant into the future at every time step.

EXAMPLE 11-8: Point transformations

Another interesting example of canonical transformations is the analogue of good old coordinate transformations. Consider the case of a two-dimensional phase space and a coordinate transformation

$$Q = f(q). \tag{11.106}$$

For this to be a canonical transformation, we need to transform the associated momenta in a specific way. We may use

$$F_2 = f(q)P \Rightarrow p = \frac{\partial f}{\partial q}P\ . \tag{11.107}$$

Hence, as long as we transform the momenta as

$$p = \frac{\partial f}{\partial q}P \tag{11.108}$$

we are guaranteed that the transformation is canonical.

11.5 Poisson brackets

Identifying the Hamiltonian as a generator of infinitesimal canonical transformations suggests that the interesting structure of phase space lies in general canonical transformations. We can view this in analogy to Lorentz symmetry in coordinate space. We had learned in Chapter 2 that the invariance of the metric or line element

$$ds^2 = -c^2dt^2 + dx^2 + dy^2 + dz^2 \tag{11.109}$$

played a central role in defining Lorentz transformations; and the invariance of the laws of the physics under the latter was a hallmark of the laws of mechanics. In the Hamiltonian picture, our playground is phase space; and canonical transformations play an equally central role in prescribing dynamics there, as we have just learned. What is then the invariant object in phase space – the analogue of the "metric" – which is left invariant under canonical transformations? Such a mathematical object is bound to package a great deal of the structure of Hamiltonian dynamics.

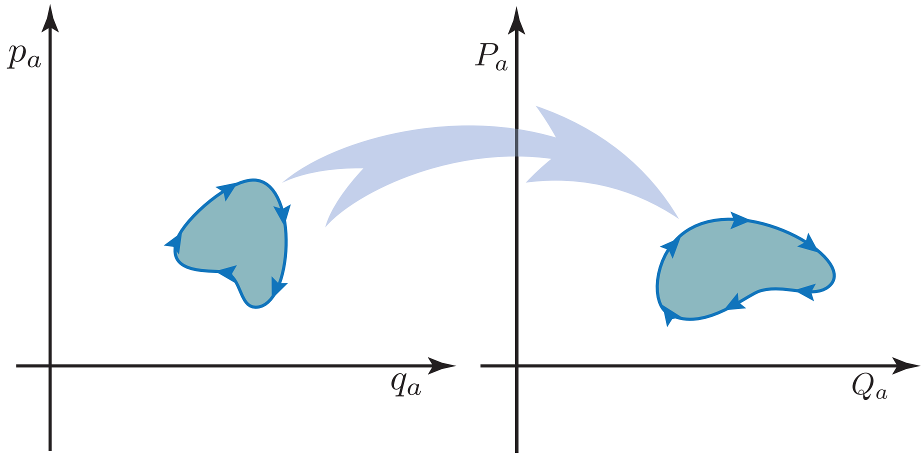

FIGURE 11.8 : The transformation of phase space under a canonical transformation. Volume elements may get distorted in shape, but the volume of each element must remain unchanged.

Consider a $2N$ dimensional phase space parameterized by $\{q_k, p_k\}$. A canonical transformation generated by $F_1(q_a, Q_a)$ relabels phase space with $\{Q_k, P_k\}$. Here, q_a is one of the many q_k's, and Q_a is one of the Q_k's. Focus on this particular q_a,p_a plane as shown in Figure 11.8. The line integral over a closed path in this space of dF_1 must vanish because the path is closed; that is,

$$\oint dF_1 = 0. \tag{11.110}$$

But we also can write

$$\begin{aligned}\oint dF_1 &= \oint \frac{\partial F_1}{\partial q_a} dq_a + \frac{\partial F_1}{\partial Q_a} dQ_a \\ &= \oint p_a dq_a - P_a dQ_a \quad \text{(no sum over } a\text{)}\end{aligned} \tag{11.111}$$

using equation (11.94). This implies

$$\oint p_a dq_a = \oint P_a dQ_a \Rightarrow \int dp_a dq_a = \int dP_a dQ_a \quad \text{(no sum over } a\text{)} \tag{11.112}$$

where in the last step we used Stokes's theorem relating a line integral over a closed path in two dimensions to the area integral over the area enclosed by the path,

$$\oint \psi \boldsymbol{dl} = \int \hat{\boldsymbol{n}} \times \boldsymbol{\nabla} \psi dA \Rightarrow \oint \psi(p) dq = \int \frac{d\psi}{dp} dp dq\ . \tag{11.113}$$

To see this, write $\boldsymbol{dl} = dq\,\hat{\boldsymbol{q}} + dp\,\hat{\boldsymbol{p}}$ where $\hat{\boldsymbol{q}}$ and $\hat{\boldsymbol{p}}$ are unit vectors in the direction of increasing q and p respectively, and note that the orientation of the path is synced with the orientation of the area normal $\hat{\boldsymbol{n}} = \hat{\boldsymbol{p}} \times \hat{\boldsymbol{q}}$. Since the closed path is arbitrary, and hence the enclosed area is arbitrary, equation (11.112)) implies that canonical transformations preserve area in phase space (see Figure 11.8. Equivalently, the *measure* in phase space must be invariant,

$$dp_a dq_a = dP_a dQ_a = \text{Det}\left[\frac{\partial(P_a, Q_a)}{\partial(p_a, q_a)}\right] dp_a dq_a \quad (\text{no sum over } a) \tag{11.114}$$

where on the right we have written the Jacobian of the corresponding canonical transformation

$$\text{Jacobian} = \text{Det}\left[\frac{\partial(P_a, Q_a)}{\partial(p_a, q_a)}\right] = 1 \quad (\text{no sum over } a) \tag{11.115}$$

which must equal unity if canonical transformations are to preserve phase space area. We remind the reader that the transformation matrix $\partial(A, B)/\partial(x, y)$ with two functions $A(x, y)$ and $B(x, y)$ is defined as

$$\frac{\partial(A, B)}{\partial(x, y)} \equiv \begin{pmatrix} \partial A/\partial x & \partial A/\partial y \\ \partial B/\partial x & \partial B/\partial y \end{pmatrix}. \tag{11.116}$$

Let us introduce a new notation, the so-called **Poisson bracket**:[4]

$$\{A, B\}_{\mathrm{x,y}} \equiv \text{Det}\left[\frac{\partial(A, B)}{\partial(x, y)}\right] \tag{11.117}$$

For example, we can then write equation (11.115) as

$$\{P_a, Q_a\}_{\mathrm{q_a,p_a}} = 1 \quad \text{no sum over } a \tag{11.118}$$

We can extend our argument to different combinations of q_a,p_a pairs in the full $2N$ dimensional phase space (see exercises at the end of the chapter), and we conclude that canonical transformations preserve phase space "volume"

$$dq_1 dp_1 dq_2 dp_2 \cdots dq_k dp_k = dQ_1 dP_1 dQ_2 dP_2 \cdots dQ_k dP_k\ . \tag{11.119}$$

We then write the Poisson bracket of two functions $A(q, p)$ and $B(q, p)$ in $2N$ dimensional phase space as

$$\{A, B\}_{\mathrm{q,p}} \equiv \frac{\partial A}{\partial q_k}\frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k}\frac{\partial B}{\partial q_k} \tag{11.120}$$

[4]Named for the French mathematician and physicist Simeon Denis Poisson (1781-1840).

where we have now extended the definition to $2N$ dimensions by summing over all two dimensional subspaces labeled by q_k, p_k (since the index k is repeated in this expression). One can now show that canonical transformations preserve this generalized Poisson bracket; that is

$$\{A, B\}_{\rm q,p} = \{A, B\}_{\rm Q,P} \ . \tag{11.121}$$

The equivalent of the metric invariant of Lorentz transformations in phase space is hence the phase space integration measure (11.119)); or equivalently the differential operator from (11.120

$$\frac{\partial}{\partial q_k}\frac{\partial}{\partial p_k} - \frac{\partial}{\partial p_k}\frac{\partial}{\partial q_k} = \frac{\partial}{\partial Q_k}\frac{\partial}{\partial P_k} - \frac{\partial}{\partial P_k}\frac{\partial}{\partial Q_k}. \tag{11.122}$$

Reversing the statement, it is also possible to show that all phase space transformations that preserve the measure (11.119)), or equivalently the Poisson bracket (11.120, are canonical transformations. For example, we can use the preservation of Poisson brackets as a test of the canonicality of a transformation.

EXAMPLE 11-9: Position and momenta

Using (11.120), one can easily show that the Poisson brackets of the $p's$ and $q's$ are

$$\{p_a, q_b\}_{\rm q,p} = \frac{\partial p_a}{\partial q_k}\frac{\partial q_b}{\partial p_k} - \frac{\partial p_a}{\partial p_k}\frac{\partial q_b}{\partial q_k} = \delta_{\rm ab} \ ; \tag{11.123}$$

that is, p_a and q_b “Poisson commute” for $a \neq b$; if $a = b$, the result is unity. We can similarly see that

$$\{q_a, q_b\}_{\rm q,p} = \{p_a, p_b\}_{\rm q,p} = 0 \ . \tag{11.124}$$

Given a candidate canonical transformation $Q_k(q, p, t)$ and $P_k(q, p, t)$, we can *test* for canonicality by verifying that

$$\{P_a, Q_b\}_{\rm q,p} = \delta_{\rm ab} \quad , \quad \{Q_a, Q_b\}_{\rm q,p} = \{P_a, P_b\}_{\rm q,p} = 0 \tag{11.125}$$

since

$$\begin{aligned} \{P_a, Q_b\}_{\rm q,p} &= \{p_a, q_b\}_{\rm q,p} \\ \{Q_a, Q_b\}_{\rm q,p} &= \{q_a, q_b\}_{\rm q,p} \\ \{P_a, P_b\}_{\rm q,p} &= \{p_a, p_b\}_{\rm q,p} \end{aligned} \tag{11.126}$$

for canonical transformations. That this is *sufficient* for demonstrating that the Poisson bracket of any two functions in phase space is preserved by the candidate transformation is left as an exercise at the end of this chapter.

EXAMPLE 11-10: The simple harmonic oscillator once again

Consider the simple harmonic oscillator from (11.72), with Hamiltonian

$$H = \frac{p^2}{2\,m} + \frac{1}{2} m\omega^2 q^2 \; . \tag{11.127}$$

The structure of the Hamiltonian as a sum of squares suggests a transformation of the form

$$q(Q,P) \propto \sqrt{\frac{2}{m\,\omega^2}} \sin Q \quad , \quad p(Q,P) \propto \sqrt{2\,m} \cos Q \; , \tag{11.128}$$

since the identity $\cos^2 Q + \sin^2 Q = 1$ would simplify the new Hamiltonian $\widetilde{H}$. Let us try to transform to a new Hamiltonian that looks like

$$\widetilde{H} = \omega P \; . \tag{11.129}$$

This would be interesting, since the equations of motion would then imply

$$\dot{Q} = \frac{\partial \widetilde{H}}{\partial P} = \omega \quad , \quad \dot{P} = -\frac{\partial \widetilde{H}}{\partial Q} = 0 \; , \tag{11.130}$$

which can immediately be solved, yielding

$$Q(t) = \omega t + Q_0 \quad , \quad P(t) = P_0 \; . \tag{11.131}$$

To achieve this transformation, we write

$$q(Q,P) = \sqrt{\frac{2P}{m\omega}} \sin Q \quad , \quad p(Q,P) = \sqrt{2m\omega P} \cos Q \tag{11.132}$$

according to equation (11.128)). But is this a canonical transformation? If not, we would not have the evolution equations given by (11.130. To test for canonicality, we check the Poisson bracket

$$\{q,p\}_{\mathrm{q,p}} = 1 = \{q,p\}_{\mathrm{Q,P}} = \left\{ \sqrt{\frac{2P}{m\omega}} \sin Q, \sqrt{2m\omega P} \cos Q \right\}_{\mathrm{Q,P}} \; . \tag{11.133}$$

Using the definition (11.120)), we indeed verify, after some algebra, that this holds. Similarly, we can show that $\{q,q\}_{\mathrm{Q,P}} = \{p,p\}_{\mathrm{Q,P}} = 0$. With these three statements, we conclude that the transformation (11.132) is indeed canonical. Substituting the solution (11.131) in (11.132, we find the solution in the original variables

$$q(Q,P)=\sqrt{\frac{2P_0}{m\omega}}\sin\omega t+Q_0 \quad , \quad p(Q,P)=\sqrt{2m\omega P_0}\cos\omega t+Q_0 \ , \tag{11.134}$$

which should now look familiar. We have thus demonstrated a new strategy of tackling a dynamical system: first attempt to find/guess at a canonical transformation to simplify the Hamiltonian; and then verify the canonicality using the Poisson bracket. Sometimes guessing at a strategic canonical transformation turns out to be easier than tackling the original Hamiltonian in its full glory. ———

In the exercises at the end of the chapter, we explore some of the most important properties of Poisson brackets. In particular, one can show the following identities that follow from the definition (11.120)

$$\{A,B\}_{\mathrm{q,p}}=-\{B,A\}_{\mathrm{q,p}} \ , \qquad \text{Anticommutativity} \tag{11.135}$$

$$\{A,B+C\}_{\mathrm{q,p}}=\{A,B\}_{\mathrm{q,p}}+\{A,C\}_{\mathrm{q,p}} \ , \qquad \text{Distributivity} \tag{11.136}$$

and, most interestingly, the *Jacobi identity*

$$\left\{A,\{B,C\}_{\mathrm{q,p}}\right\}_{\mathrm{q,p}}+\left\{B,\{C,A\}_{\mathrm{q,p}}\right\}_{\mathrm{q,p}}+\left\{C,\{A,B\}_{\mathrm{q,p}}\right\}_{\mathrm{q,p}}=0. \tag{11.137}$$

We can also use the Poisson bracket to write Hamilton's equations of motion as

$$\dot{q}=\{q,H\}_{\mathrm{q,p}} \quad , \quad \dot{p}=\{p,H\}_{\mathrm{q,p}} \tag{11.138}$$

as can be easily verified using (11.120). This makes explicit the fact that canonical transformations do not change the structural form of Hamilton's equations. More generally, we can write

$$\frac{dA}{dt}=\frac{\partial A}{\partial t}+\{A,H\}_{\mathrm{q,p}} \tag{11.139}$$

using the chain rule. Finally, for an infinitesimal transformation

$$F_2=q_kP_k+\epsilon G(q,P,t) \tag{11.140}$$

we can write

$$\begin{aligned}\delta A &= \frac{\partial A}{\partial q_k}\delta q_k+\frac{\partial A}{\partial p_k}\delta p_k=\frac{\partial A}{\partial q_k}\epsilon\frac{\partial G}{\partial p_k}-\frac{\partial A}{\partial p_k}\epsilon\frac{\partial G}{\partial q_k}\\ &= \epsilon\{A,G\}_{\mathrm{q,p}} \ .\end{aligned} \tag{11.141}$$

In short, Poisson brackets are as natural in phase space as the metric is in Minkowski space: things look simpler and more natural when written with Poisson brackets.

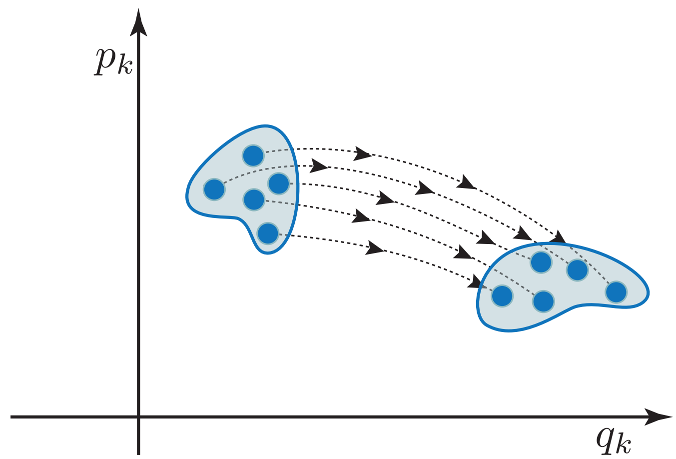

FIGURE 11.9 : A depiction of Liouville's theorem: the density of states of a system evolves in phase space in such as way that its total time derivative is zero.

11.6 Liouville's theorem

Consider a set of initial conditions in phase space whose time evolution we wish to trace, as illustrated in Figure 11.9. Let ΔN denote the number of such initial conditions, and ΔV the volume of phase space they start out occupying. The density of such initial conditions is then

$$\rho(q, p, t) = \frac{\Delta N}{\Delta V} \ . \tag{11.142}$$

As time evolves, ΔN remains unchanged since any state of the system is not to suddenly disappear as we evolve in time. Furthermore, ΔV must remain unchanged by the Hamiltonian evolution: Hamiltonian evolution is a canonical transformation, and canonical transformations preserve phase space volume! The shape of the volume element may get twisted and compressed as shown in the figure, but the volume itself remains unchanged. This implies

$$\frac{d\rho}{dt} = 0 = \frac{\partial \rho}{\partial t} + \{\rho, H\}_{\mathrm{q,p}} \Rightarrow \frac{\partial \rho}{\partial t} = -\{\rho, H\}_{\mathrm{q,p}} \tag{11.143}$$

using equation (11.139). This is known as **Liouville's theorem**:[5] the density of states in phase space remains constant in time! Liouville's theorem

[5]Named for the French mathematician Joseph Liouville (1809-1882).

plays an important role in statistical mechanics and fluid dynamics. It also packages within it the seeds of quantization, as we shall see at the end of this part of the book. We leave further exploration of the theorem to exercises and to Chapter 14.4.

Problems

PROBLEM 11-1: Find the Legendre transform $B(x,z)$ of the function $A(x,y) = x^4 - (y+a)^4$, and verify that $-\partial A/\partial x = \partial B/\partial x$.

PROBLEM 11-2: In thermodynamics the enthalpy H (no relation to the Hamiltonian H) is a function of the entropy S and pressure P such that $\partial H/\partial S = T$ and $\partial H/\partial P = V$, so that

$$dH = TdS + VdP$$

where T is the temperature and V the volume. The enthalpy is particularly useful in isentropic and isobaric processes, because if the process is isentropic or isobaric, one of the two terms on the right vanishes. But suppose we wanted to deal with *isothermal* and isobaric processes, by constructing a function of T and P alone. Define such a function, in terms of H, T, and S, using a Legendre transformation. (The defined function G is called the Gibbs free energy.)

PROBLEM 11-3: In thermodynamics, for a system such as an enclosed gas, the internal energy $U(S,V)$ can be expressed in terms of the independent variables of entropy S and volume V, such that $dU = TdS - PdV$, where T is the temperature and P the pressure. Suppose we want to find a related function in which the volume is to be eliminated in favor of the pressure, using a Legendre transformation. (a) Which is the passive variable, and which are the active variables? (b) Find an expression for the new function in terms of U, P, and V. (The result is the enthalpy H or its negative, where the enthalpy H is unrelated to the Hamiltonian H.)

PROBLEM 11-4: The kinetic energy of a relativistic free particle is the Hamiltonian $H = \sqrt{p^2c^2 + m^2c^4}$ in terms of the particle's momentum and mass. (a) Using one of Hamilton's equations in one dimension, find the particle's velocity v in terms of its momentum and mass. (b) Invert the result to find the momentum p in terms of the velocity and the mass. (c) Then find the free-particle Lagrangian for a relativistic particle using the Legendre transform

$$L(v) = pv - H.$$

(d) Beginning with the same Hamiltonian, generalize parts (a), (b). and (c) to a relativistic particle free to move in three dimensions.

PROBLEM 11-5: The Lagrangian for a particular system is

$$L = \dot{x}^2 + b\dot{y} + c\dot{x}\dot{z} + d\frac{\dot{z}}{y^2} - ex^2y^2,$$

where a, b, c, d, and e are constants. Find the Hamiltonian, identify any conserved quantities, and write out Hamilton's equations of motion.

PROBLEM 11-6: A system with two degrees of freedom has the Lagrangian

$$L = \dot{q}_1^2 + \frac{\dot{q}_1^2 + \dot{q}_2^2}{1 + q_2^2} + \alpha\dot{q}_1\dot{q}_2 + \beta q_2^2/2,$$

where α, and β are constants. Find the Hamiltonian, identify any conserved quantities, and write out Hamilton's equations of motion.

PROBLEM 11-7: Write the Hamiltonian and find Hamilton's equations of motion for a simple pendulum of length ℓ and mass m. Sketch the constant-H contours in the θ, p_θ phase plane.

PROBLEM 11-8: (a) Write the Hamiltonian for a spherical pendulum of length ℓ and mass m, using the polar angle θ and azimuthal angle φ as generalized coordinates. (b) Then write out Hamilton's equations of motion, and identify two first-integrals of motion. (c) Find a first-order differential equation of motion involving θ alone and its first time derivative. (d) Sketch contours of constant H in the θ, p_θ phase plane, and use it to identify the types of motion one expects.

PROBLEM 11-9: A Hamiltonian with one degree of freedom has the form

$$H = \frac{p^2}{2m} + \frac{kq^2}{2} + aqp - 2bq^3 \sin \alpha t$$

where $m, k, a, b,$ and α are constants. Find the Lagrangian corresponding to this Hamiltonian. Write out both Hamilton's equations and Lagrange's equations, and show directly that they are equivalent.

PROBLEM 11-10: A particle of mass m slides on the inside of a frictionless vertically-oriented cone of semi-vertical angle α. Find the Hamiltonian H of the particle, using generalized coordinates r, the distance from the vertex, and φ, the azimuthal angle. (a) SHow that stable circular motion is possible for any value of r, and find the corresponding angular velocity ω. (b) Find the frequency of small oscillations about this circular motion, and compare it with ω.

PROBLEM 11-11: A particle of mass m is attracted to the origin by a force of magnitude k/r^2. Using plane polar coordinates, find the Hamiltonian and Hamilton's equations of motion. Sketch constant-H contours in the (r, p_r) phase plane.

PROBLEM 11-12: A double pendulum consists of two strings and two bobs. The upper string, of length ℓ_1, is attached to the ceiling, while the lower end is attached to a bob of mass m_1. One end of the lower string, of length ℓ_2, is attached to m_1, while the other end is attached to the bob of mass m_2. Using generalized coordinates θ_1 (the angle of the upper string relative to the vertical) and θ_2 (the angle of the lower string relative to the vertical), find the Hamiltonian and Hamilton's equations of motion. Are there any constants of the motion? If so, what are they, and why are they constants?

PROBLEM 11-13: A double Atwood's machine consists of two massless pulleys, each of radius R, some massless string, and three weights, with masses m_1, m_2, and m_3. The axis of pulley 1 is supported by a strut from the ceiling. A piece is string of length ℓ_1 is slung over the pulley, and one end of the string is attached to weight m_1 while the other end is attached to the axis of pulley 2. A second string of length ℓ_2 is slung over pulley 2; one end is attached to m_2 and the other to m_3. The strings are inextendible, but otherwise the weights and pulley

2 are free to move vertically. Let x be the distance of m_1 below the axis of pulley 1, and y be the distance of m_2 below the axis of pulley 2. Find the Hamiltonian of the system, write down Hamilton's equations, and use them to find the motion $x(t)$ and $y(t)$ of the system.

PROBLEM 11-14: A massless unstretchable string is slung over a massless pulley. A weight of mass $2m$ is attached to one end of the string and a weight of mass m is attached to the other end. One end of a spring of force constant k is attached beneath m, and a second weight of mass m is hung on the spring. Using the distance x of the weight $2m$ beneath the pulley and the stretch y of the spring as generalized coordinates, find the Hamiltonian of the system. (a) Show that one of the two coordinates is ignorable (*i.e.*, , cyclic.) To what symmetry does this correspond? (b) If the system is released from rest with $y(0) = 0$, find $x(t)$ and $y(t)$.

PROBLEM 11-15: Construct a phase-space diagram for a plane pendulum of mass m and length ℓ, with the angle θ from the vertical as generalized coordinate. (Suppose that the plumb bob swings on a massless rod rather than a string, so that the pendulum can swing all the way around while keeping ℓ constant; that is, there is no bound on θ.) Then discuss the possible types of motion using the phase-space diagram as a guide.

PROBLEM 11-16: Show directly that the transformation

$$Q = \ln\left(\frac{1}{q}\sin p\right) \qquad P = q\cot p$$

is canonical.

PROBLEM 11-17: A cyclic coordinate q_k is a coordinate absent from the Lagrangian (even though $\dot{q}_k$ is present in L.) (a) Show that a cyclic coordinate is likewise absent from the Hamiltonian. (b) Show from the Hamiltonian formalism that the momentum p_k canonical to a cyclic coordinate q_k is conserved, so $p_k = \alpha = \text{constant}$. Therefore one can ignore both q_k and p_k in the Hamiltonian. This led E. J. Routh to suggest a procedure for dealing with problems having cyclic coordinates. He carries out a transformation from the $q, \dot{q}$ basis to the q, p basis only for the cyclic coordinates, finding their equations of motion in the Hamiltonian form, and then uses Lagrange's equations for the noncyclic coordinates. Denote the cyclic coordinates by $q_{\mathrm{s}+1}...q_n$; then define the *Routhian* as

$$R(q_1, ...q_n \ ; \ \dot{q}_1....\dot{q}_s \ ; \ p_{\mathrm{s}+1}....p_n \ ; \ t) = \sum_{\mathrm{i=s+1}}^{n} p_i\dot{q}_1 - L$$

Show then (using R rather than H) that one obtains Hamilton-type equations for the $n - s$ cyclic coordinates, while (using R rather than L) one obtains Lagrange-type equations for the non-cyclic coordinates. The Hamilton-type equations are trivial, showing that the momenta canonical to the cyclic coordinates are constants of the motion. In this procedure one can in effect "ignore" the cyclic coordinates, so "cyclic" coordinates are also "ignorable" coordinates.

PROBLEM 11-18: Show that the Poisson bracket of two constants of the motion is itself a constant of the motion, even when the constants depend explicitly on time.

PROBLEM 11-19: Show that if the Hamiltonian and some quantity Q are both constants of the motion, then the n^{th} partial derivative of Q with respect to time must also be a constant of the motion.

PROBLEM 11-20: Prove the anticommutativity and distributivity of Poisson brackets by showing that (a) $\{A, B\}_{\rm q,p} = -\{B, A\}_{\rm q,p}$ (b) $\{A, B + C\}_{\rm q,p} = \{A, B\}_{\rm q,p} + \{A, C\}_{\rm q,p}$.

PROBLEM 11-21: Prove the Jacobi identity for Poisson brackets,

$$\Big\{A, \{B, C\}_{\rm q,p}\Big\}_{\rm q,p} + \Big\{B, \{C, A\}_{\rm q,p}\Big\}_{\rm q,p} + \Big\{C, \{A, B\}_{\rm q,p}\Big\}_{\rm q,p} = 0.$$

PROBLEM 11-22: Show that Hamilton's equations of motion can be written in terms of Poisson brackets as

$$\dot{q} = \{q, H\}_{\rm q,p} \ , \quad \dot{p} = \{p, H\}_{\rm q,p} \, .$$

PROBLEM 11-23: A Hamiltonian has the form

$$H = q_1 p_1 - q_2 p_2 + a q_1^2 - b q_2^2,$$

where a and b are constants. (a) Using the method of Poisson brackets, show that

$$f_1 \equiv q_1 q_2 \quad \text{and} \quad f_2 \equiv \frac{1}{q_1}(p_2 + b q_2)$$

are constants of the motion. (b) Then show that $[f_1, f_2]$ is also a constant of the motion. (c) Is H itself constant? Check by finding $q_1, q_2, p_1,$ and p_2 as explicit functions of time.

PROBLEM 11-24: Show, using the Poisson bracket formalism, that the *Laplace-Runge-Lenz vector*

$$\boldsymbol{A} \equiv \boldsymbol{p} \ \times \ \boldsymbol{L} - \frac{mk\boldsymbol{r}}{r}$$

is a constant of the motion for the Kepler problem of a particle moving in the central inverse-square force field $F = -k/r^2$. Here $\boldsymbol{p}$ is the particle's momentum, and $\boldsymbol{L}$ is its angular momentum.

PROBLEM 11-25: A beam of protons having a circular cross-section of radius r_0 moves within a linear accelerator oriented in the x direction. Suppose that the transverse momentum components (p_y, p_z) of the beam are distributed uniformly in momentum space, in a circle of radius p_0. If a magnetic lens system at the end of the accelerator focusses the beam into a small circular spot of radius r_1, find, using Liouville's theorem, the corresponding distribution of the beam in momentum space. Here what may be a desirable focussing of the beam in position-space has the often unfortunate consequence of broadening the momentum distribution.

PROBLEM 11-26: A large number of particles, each of mass m, move in response to a uniform gravitational field g in the negative z direction. At time $t = 0$, they are all located within the corners of a rectangle in (z, p_z) phase space, whose positions are: (1) $z = z_0, p_z = p_0$, (2) $z = z_0 + \Delta z, p_z = p_0$, (3) $z = z_0, p_z = p_0 + \Delta p$, and (4) $z = z_0 + \Delta z, p_z = p_0 + \Delta p$. By direct computation, find the area in phase space enclosed by these particles at times (a) $t = 0, (b) t = m\Delta z/p_0$, and (c) $t = 2m\Delta z/p_0$. Also show the shape of the region in phase space for cases (b) and (c).

PROBLEM 11-27: In an electron microscope, electrons scattered from an object of height z_0 are focused by a lens at distance D_0 from the object and form an image of height z_1 at a distance D_1 behind the lens. The aperture of the lens is A. Show by direct calculation that the area in the (z, p_z) phase plane occupied by electrons leaving the object (and destined to pass through the lens) is the same as the phase area occupied by electrons arriving at the image. Assume that $z_0 \ll D_0$ and $z_1 \ll D_1$. (from *Mechanics*, 3rd edition, by Keith R. Symon.)

Leonhard Euler (1707 - September 1783)

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