Hamiltonian Mechanics

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1 Phase space

Phase space is a dynamical arena for classical mechanics in which the number of independent dynamical variables variables, q_i, $i = 1, 2, \ldots, n$, is doubled from n to $2n$ by treating either the velocities or the momenta as independent variables. This has three important consequences.

First, the equations of motion become first order differential equations instead of second order, so that the initial conditions specify a single point, $(\mathbf{x}_0, \mathbf{p}_0)$ in phase space. In the Newtonian treatment, through any point $\mathbf{x}_0$ there are still many solutions corresponding to different initial velocities. In phase spaces, however, points are in 1-1 correspondence with initial conditions, so there is a unique solution to the equations of motion through each point. This permits some useful geometric techniques in the study of even very complicated systems, even chaotic ones.

Second, as we shall see, the set of transformations that preserve the equations of motion is enlarged. In Lagrangian mechanics, we are free to use n general coordinates, q_i, for our description. In phase space we have $2n$ coordinates. Even though transformations among these $2n$ coordinates are not completely arbitrary, there are far more allowed transformations. This large set of transformations allows us, at least formally, to write a general solution to mechanical problems via the Hamilton-Jacobi equation.

Finally, quantum mechanics requires configuration and momentum variables to be on an equal footing (consider, for example, the uncertainty relation, $\Delta x \Delta p \geq \frac{\hbar}{2}$). Phase space provides the right arena for this equality. It is not surprising that the closest approach of classical mechanics to quantum mechanics occurs in the Hamiltonian formulation.

1.1 Velocity phase space

While we will not be using velocity phase space here, it provides some motivation for our developments in the next Sections. The formal presentation of Hamiltonian dynamics begins in Section 1.3.

Suppose we have an action functional

$$S = \int L\left(q_i, \dot{q}_j, t\right) dt$$

dependent on n dynamical variables, $q_i(t)$, and their time derivatives. We might instead treat $L(q_i, u_j, t)$ as a function of $2n$ dynamical variables. Thus, instead of treating the the velocities as time derivatives of the position variables, $(q_i, \dot{q}_i)$ we introduce n velocities u_i and treat them as independent. Then the variations of the velocities δu_i are also independent, and we end up with $2n$ equations. Finally, we include n constraints, restoring the relationship between q_i and $\dot{q}_i$,

$$S = \int \left[L\left(q_i, u_j, t\right) + \sum \lambda_i \left(\dot{q}_i - u_i\right)\right] dt$$

Now vary the $2n$ independent variables and the Lagrange multipliers. For the coordinates, q_i,

$$\begin{aligned} 0 &= \delta_q S \\ &= \int \left(\frac{\partial L}{\partial q_i}\delta q_i + \lambda_i \delta \dot{q}_i\right) dt \\ &= \int \left(\frac{\partial L}{\partial q_i} - \dot{\lambda}_i\right) \delta q_i dt \end{aligned}$$

so that

$$\dot{\lambda}_i = \frac{\partial L}{\partial q_i} \tag{1}$$

For the velocities, we find

$$\begin{aligned} 0 &= \delta_u S \\ &= \int \left(\frac{\partial L}{\partial u_i} - \lambda_i\right) \delta u_i dt \end{aligned}$$

so that

$$\lambda_i = \frac{\partial L}{\partial u_i} \tag{2}$$

and finally, varying the Lagrange multipliers, λ_i, we recover the constraints,

$$u_i = \dot{q}_i \tag{3}$$

We may eliminate the multipliers by differentiating the velocity equation

$$\frac{d}{dt}(\lambda_i) = \frac{d}{dt}\left(\frac{\partial L}{\partial u_i}\right)$$

to find $\dot{\lambda}_i$, then substituting this result for $\dot{\lambda}_i$ into the Eq.(1)

$$\dot{\lambda}_i = \frac{d}{dt}\left(\frac{\partial L}{\partial u_i}\right) = \frac{\partial L}{\partial q_i}$$

Now, using the constraint to set $u_i = \dot{q}_i$, we recover the Euler-Lagrange equation,

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

If the kinetic energy is of the form $\sum_{i=1}^{n} \frac{1}{2} m u_i^2$, then the Lagrange multipliers are just the Newtonian momenta,

$$\begin{aligned} \lambda_i &= \frac{\partial L}{\partial u_i} \\ &= m u_i \\ &= m \dot{q}_i \end{aligned}$$

The space of all positions and velocities, $\left\{\left(x^i, v^i\right)\right\}$, is called *velocity phase space*.

1.2 Phase space

We can make the construction above more general by requiring the Lagrange multipliers to *always* be the conjugate momenta. Combining the constraint equation with the equation for λ_i we have

$$\lambda_i = \frac{\partial L}{\partial \dot{q}_i}$$

and we have defined the conjugate momentum to be exactly this derivative,

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$$

Then the action becomes

$$\begin{aligned} S &= \int \left[L\left(q_i, u_j, t\right) + \sum p_i\left(\dot{q}_i - u_i\right)\right] dt \\ &= \int \left[L\left(q_i, u_j, t\right) - \sum p_i u_i + \sum p_i \dot{q}_i\right] dt \end{aligned}$$

For Lagrangians quadratic in the velocities, the first two terms become

$$\begin{aligned} L\left(q_i, u_j, t\right) - \sum p_i u_i &= L\left(q_i, \dot{q}, t\right) - \sum p_i \dot{q}_i \\ &= T - V - \sum p_i \dot{q}_i \\ &= -\left(T + V\right) \end{aligned}$$

For Lagrangians with no explicit time dependence, this is just the negative of the conserved energy, but whether it is conserved or not, we now define the *Hamiltonian* to be

$$H \equiv \sum p_i \dot{q}_i - L\left(q_i, \dot{q}, t\right) \tag{4}$$

Then we may write the Lagrangian as

$$S = \int \left[\sum p_i \dot{q}_i - H\right] dt$$

This successfully eliminates the Lagrange multipliers from the formulation.

The term "phase space" is generally reserved for momentum phase space, spanned by coordinates q_i, p_j.

1.2.1 Legendre transformation

Notice that $H = \sum p_j \dot{q}_j - L$ is, by definition, independent of the velocities, since

$$\begin{aligned}
\frac{\partial H}{\partial \dot{q}_i} &= \frac{\partial}{\partial \dot{q}_i}\left(\sum_j p_j \dot{q}_j - L\right) \\
&= \sum_j p_j \delta_{ij} - \frac{\partial L}{\partial \dot{q}_i} \\
&= p_i - \frac{\partial L}{\partial \dot{q}_i} \\
&\equiv 0
\end{aligned}$$

Therefore, the Hamiltonian is a function of q_i and p_i only. This is an example of a general technique called *Legendre transformation*. Suppose we have a function f, which depends on independent variables A, B and dependent variables, having partial derivatives

$$\begin{aligned}
\frac{\partial f}{\partial A} &= P \\
\frac{\partial f}{\partial B} &= Q
\end{aligned}$$

Then the differential of f is

$$df = PdA + QdB$$

A Legendre transformation allows us to interchange variables to make either P or Q or both into the independent variables. For example, let $g\left(A, B, P\right) \equiv f - PA$. Then

$$\begin{aligned}
dg &= df - AdP - PdA \\
&= PdA + QdB - AdP - PdA \\
&= QdB - AdP
\end{aligned}$$

so that g actually only changes with B and P, $g = g\left(B, P\right)$. Similarly, $h = f - QB$ is a function of $\left(A, Q\right)$ only, while $k = -\left(f - PA - QB\right)$ has $\left(P, Q\right)$ as independent variables. Explicitly,

$$\begin{aligned}
dk &= -df + PdA + AdP + QdB + BdQ \\
&= AdP + BdQ
\end{aligned}$$

and we now have

$$\begin{aligned}
\frac{\partial f}{\partial P} &= A \\
\frac{\partial f}{\partial Q} &= B
\end{aligned}$$

Legendre transformations are familiar from thermodynamics, where the internal energy $U(S,V)$ is given by the second law,

$$dU = TdS - PdV$$

It may be altered by a Legendre transformation to give the Helmholz free energy, $A = U - TS$, the enthalpy, $H(S,P) = U + PV$, or the the Gibbs free energy, $g(T,P) = U - TS + PV$.

We now see that writing

$$H = \sum_j p_j \dot{q}_j - L$$

is simply a Legendre transformation of the Lagrangian that replaces the momenta p_i in place of the velcities $\dot{q}_i$ as independent variables.

2 Hamilton's equations

The essential formalism of Hamiltonian mechanics is as follows. We begin with the action

$$S = \int L(q_i, \dot{q}_j, t)\, dt$$

and define the conjugate momenta

$$p_i \equiv \frac{\partial L}{\partial \dot{q}_i}$$

and Hamiltonian

$$H(q_i, p_j, t) \equiv \sum p_j \dot{q}_j - L(q_i, \dot{q}_j, t)$$

Then the action may be written as

$$S = \int \left[\sum p_j \dot{q}_j - H(q_i, p_j, t)\right] dt$$

where q_i and p_j are now treated as the independent variables.

Finding extrema of the action with respect to all $2n$ variables, we find for the coordinate variation,

$$\begin{aligned}
0 &= \delta_{q_k} S \\
&= \int \left(\left(\frac{\partial}{\partial \dot{q}_k} \sum_j p_j \dot{q}_j \right) \delta \dot{q}_k - \frac{\partial H}{\partial q_k} \delta q_k \right) dt \\
&= \int \left(\sum_j p_j \delta_{jk} \delta \dot{q}_k - \frac{\partial H}{\partial q_k} \delta q_k \right) dt \\
&= \int \left(p_k \delta \dot{q}_k - \frac{\partial H}{\partial q_k} \delta q_k \right) dt \\
&= \int \left(-\dot{p}_k - \frac{\partial H}{\partial q_k} \right) \delta q_k dt
\end{aligned}$$

where we have discarded a surface term. Then

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

For the momentum variation,

$$\begin{aligned}
0 &= \delta_{pk} S \\
&= \int \left(\left(\frac{\partial}{\partial p_k} \sum_j p_j \dot{q}_j \right) \delta p_k - \frac{\partial H}{\partial p_k} \delta p_k \right) dt \\
&= \int \left(\dot{q}_k \delta p_k - \frac{\partial H}{\partial p_k} \delta p_k \right) dt \\
&= \int \left(\dot{q}_k - \frac{\partial H}{\partial p_k} \right) \delta p_k dt
\end{aligned}$$

and we conclude that

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

These are *Hamilton's equations.* Whenever the Legendre transformation between L and H and between $\dot{q}_k$ and p_k is non-degenerate, Hamilton's equations,

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \tag{5}$$

$$\dot{p}_k = -\frac{\partial H}{\partial q_k} \tag{6}$$

form a system equivalent to the Euler-Lagrange equation or Newton's second law.

2.1 Example: Newton's second law

Suppose the Lagrangian takes the familiar form

$$L = \frac{1}{2} m \dot{\mathbf{x}}^2 - V(\mathbf{x})$$

Then the conjugate momenta are

$$\begin{aligned}
p_i &= \frac{\partial L}{\partial \dot{x}_i} \\
&= m \dot{x}_i
\end{aligned}$$

and the Hamiltonian becomes

$$\begin{aligned}
H(x_i, p_j, t) &\equiv \sum p_j \dot{x}_j - L(x_i, \dot{x}_j, t) \\
&= m \dot{\mathbf{x}}^2 - \frac{1}{2} m \dot{\mathbf{x}}^2 + V(\mathbf{x}) \\
&= \frac{1}{2} m \dot{\mathbf{x}}^2 + V(\mathbf{x}) \\
&= \frac{1}{2m} \mathbf{p}^2 + V(\mathbf{x})
\end{aligned}$$

Notice that we must invert the relationship between the momenta and the velocities,

$$\dot{x}_i = \frac{p_i}{m}$$

then expicitly replace all occurrences of the velocity with appropriate combinations of the momentum.

Hamilton's equations are:

$$\begin{aligned}
\dot{x}_k &= \frac{\partial H}{\partial p_k} \\
&= \frac{p_k}{m} \\
\dot{p}_k &= -\frac{\partial H}{\partial x_k} \\
&= -\frac{\partial V}{\partial x_k}
\end{aligned}$$

If we take a second time derivative of $\dot{x}_k$, to give $m\ddot{x}_k = \dot{p}_k$, and substitute into the second, we have

$$-\frac{\partial V}{\partial x_k} = m\ddot{x}_k$$

thereby reproducing the usual definition of momentum and Newton's second law.

2.2 Example: coupled oscillators

Suppose we have coupled oscillators comprised of two identical pendula of length l and each of mass m, connected by a light spring with spring constant k. Let the first pendulum be displaced through an angle θ_1 and the second through θ_2. Then since the potential of the spring is

$$\begin{aligned}
\frac{1}{2}k\left(\triangle x^2 + \triangle y^2\right) &= \frac{1}{2}k\left((l\sin\theta_1 - l\sin\theta_2)^2 + (l\cos\theta_1 - l\cos\theta_2)^2\right) \\
&= \frac{1}{2}kl^2\left(\sin^2\theta_1 - 2\sin\theta_1\sin\theta_2 + \sin^2\theta_2 + \cos^2\theta_1 - 2\cos\theta_1\cos\theta_2 + \cos^2\theta_2^2\right) \\
&= kl^2\left(1 - \sin\theta_1\sin\theta_2 - \cos\theta_1\cos\theta_2\right) \\
&= kl^2\left(1 - \cos\left(\theta_1 - \theta_2\right)\right)
\end{aligned}$$

the action becomes

$$S = \int\left[\frac{1}{2}ml^2\left(\dot{\theta}_1^2 + \dot{\theta}_2^2\right) - kl^2\left(1 - \cos\left(\theta_1 - \theta_2\right)\right) - mgl\left(1 - \cos\theta_1\right) - mgl\left(1 - \cos\theta_2\right)\right]dt$$

For small angles we approximate $\cos\theta \approx 1 - \frac{1}{2}\theta^2$ and the action becomes approximately

$$S = \int\left[\frac{1}{2}ml^2\left(\dot{\theta}_1^2 + \dot{\theta}_2^2\right) - \frac{1}{2}kl^2\left(\theta_1 - \theta_2\right)^2 - \frac{1}{2}mgl\left(\theta_1^2 + \theta_2^2\right)\right]dt$$

The conjugate momenta are,

$$\begin{aligned}
p_1 &= \frac{\partial L}{\partial \dot{\theta}_1} \\
&= ml^2\dot{\theta}_1 \\
p_2 &= \frac{\partial L}{\partial \dot{\theta}_2} \\
&= ml^2\dot{\theta}_2
\end{aligned}$$

so we may compute

$$\begin{aligned}
H &= p_1\dot{\theta}_1 + p_2\dot{\theta}_2 - L \\
&= ml^2\dot{\theta}_1^2 + ml^2\dot{\theta}_2^2 - \left(\frac{1}{2}ml^2\left(\dot{\theta}_1^2 + \dot{\theta}_2^2\right) - \frac{1}{2}kl^2\left(\theta_1 - \theta_2\right)^2 - \frac{1}{2}mgl\left(\theta_1^2 + \theta_2^2\right)\right) \\
&= \frac{1}{2}ml^2\left(\dot{\theta}_1^2 + \dot{\theta}_2^2\right) + \frac{1}{2}kl^2\left(\theta_1 - \theta_2\right)^2 + \frac{1}{2}mgl\left(\theta_1^2 + \theta_2^2\right)
\end{aligned}$$

Replacing velocities with momenta, the Hamiltonian is

$$H = \frac{1}{2ml^2}\left(p_1^2 + p_2^2\right) + \frac{1}{2}kl^2\left(\theta_1 - \theta_2\right)^2 + \frac{1}{2}mgl\left(\theta_1^2 + \theta_2^2\right) \tag{7}$$

Notice again our elimination of the velocities in favor of the momenta.

Hamilton's equations are:

$$\begin{aligned}
\dot{\theta}_1 &= \frac{\partial H}{\partial p_1} \\
&= \frac{1}{ml^2}p_1 \\
\dot{\theta}_2 &= \frac{\partial H}{\partial p_2} \\
&= \frac{1}{ml^2}p_2 \\
\dot{p}_1 &= -\frac{\partial H}{\partial \theta_1} \\
&= -kl^2\left(\theta_1 - \theta_2\right) - mgl\theta_1 \\
\dot{p}_2 &= -\frac{\partial H}{\partial \theta_2} \\
&= kl^2\left(\theta_1 - \theta_2\right) - mgl\theta_2
\end{aligned}$$

In this case, the first two equations reproduce the expressions for the momenta.

From here we may solve in any way that suggests itself. If we differentiate $\dot{\theta}_1$ again, and use the third equation, we have

$$\begin{aligned}
\ddot{\theta}_1 &= \frac{1}{ml^2}\dot{p}_1 \\
&= -\frac{k}{m}\left(\theta_1 - \theta_2\right) - \frac{g}{l}\theta_1
\end{aligned}$$

Similarly, for θ_2 we have

$$\ddot{\theta}_2 = \frac{k}{m}\left(\theta_1 - \theta_2\right) - \frac{g}{l}\theta_2$$

Subtracting,

$$\begin{aligned}
\ddot{\theta}_1 - \ddot{\theta}_2 &= -\frac{2k}{m}\left(\theta_1 - \theta_2\right) - \frac{g}{l}\left(\theta_1 - \theta_2\right) \\
\frac{d^2}{dt^2}\left(\theta_1 - \theta_2\right) + \left(\frac{2k}{m} + \frac{g}{l}\right)\left(\theta_1 - \theta_2\right) &= 0
\end{aligned}$$

so that

$$\theta_1 - \theta_2 = A\sin\omega_1 t + B\cos\omega_1 t$$

with

$$\omega_1 = \sqrt{\frac{2k}{m} + \frac{g}{l}}$$

Adding instead, we find

$$\ddot{\theta}_1 + \ddot{\theta}_2 = -\frac{g}{l}\left(\theta_1 + \theta_2\right)$$

so that

$$\theta_1 + \theta_2 = C\sin\omega_2 t + D\cos\omega_2 t$$

where $\omega_2 = \sqrt{\frac{g}{l}}$. Notice that ω_2 depends only on the gravitational restoring force since changing the total angle $\theta_1 + \theta_2$ does not stretch the spring.

The general motion is therefore a sum of two simple harmonic motions, with frequencies ω_1 and ω_2.

$$\begin{aligned}
\theta_1 &= \frac{1}{2}\left(A\sin\omega_1 t + B\cos\omega_1 t + C\sin\omega_2 t + D\cos\omega_2 t\right) \\
\theta_2 &= \frac{1}{2}\left(-A\sin\omega_1 t - B\cos\omega_1 t + C\sin\omega_2 t + D\cos\omega_2 t\right) \\
p_1 &= \frac{1}{2}ml^2\left(A\omega_1\cos\omega_1 t - B\omega_2\sin\omega_1 t + C\omega_2\cos\omega_2 t - D\omega_2\sin\omega_2 t\right) \\
p_2 &= \frac{1}{2}ml^2\left(-A\omega_1\cos\omega_1 t + B\omega_2\sin\omega_1 t + C\omega_2\cos\omega_2 t - D\omega_2\sin\omega_2 t\right)
\end{aligned}$$

The constants A, B, C, D are determined by the four initial conditions θ_{i0} and p_{i0} at time $t = 0$ by solving:

$$\begin{aligned}
\theta_{10} &= \frac{1}{2}(B + D) \\
\theta_{20} &= \frac{1}{2}(D - B) \\
p_{10} &= ml^2(\omega_1 A + \omega_2 C) \\
p_{20} &= ml^2(\omega_2 C - \omega_1 A)
\end{aligned}$$

This results in

$$\begin{aligned}
A &= \frac{p_{10}}{2ml^2\omega_1} - \frac{p_{20}}{2ml^2\omega_1} \\
B &= \theta_{10} - \theta_{20} \\
C &= \frac{p_{10}}{2ml^2\omega_2} + \frac{p_{20}}{2ml^2\omega_2} \\
D &= \theta_{10} + \theta_{20}
\end{aligned}$$

Notice that only one phase space curve, $(\theta_1, \theta_2, p_1, p_2)$ passes through the phase space point $(\theta_{10}, \theta_{20}, p_{10}, p_{20})$.

3 Conservation and cyclic coordinates

From the relationship between the Lagrangian and the Hamiltonian, $H = p_i\dot{x}_i - L$ we see that if a coordinate is cyclic in the Lagrangian it is also cyclic in the Hamiltonian,

$$\frac{\partial H}{\partial x_i} = -\frac{\partial L}{\partial x_i}$$

When a coordinate x_i is cyclic then the corresponding Hamilton equation reads

$$\dot{p}_i = -\frac{\partial H}{\partial x_i} = 0$$

and the conjugate momentum

$$p_i = \frac{\partial L}{\partial \dot{x}_i}$$

is conserved, so the relationship between cyclic coordinates and conserved quantities still holds.

Hamilton's equations show that we also have a corresponding statement about momentum. Suppose some momentum, p_i, is cyclic in the Hamiltonian,

$$\frac{\partial H}{\partial p_i} = 0$$

Then from Hamilton's equations we immediately have

$$\dot{x}_i = 0$$

so that the coordinate x_i is a constant of the motion.

Suppose we have a cyclic coordinate, say x_n. Then the conserved momentum takes its initial value, p_{n0}, and the Hamiltonian is

$$H = H\left(x_1, \ldots x_{n-1}; p_1, \ldots p_{n-1}, p_{n0}\right)$$

and therefore immediately becomes a function of $2\left(n-1\right)$ variables. This is simpler than the Lagrangian case, where constancy of p_n makes no immediate simplification of the Lagrangian.

Consider the time derivative of the Hamiltonian,

$$\begin{aligned}
\frac{dH}{dt} &= \frac{\partial H}{\partial p_i}\dot{p}_i + \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial t} \\
&= \dot{q}^i \dot{p}_i - \dot{p}_i \dot{q}^i + \frac{\partial H}{\partial t} \\
&= \frac{\partial H}{\partial t}
\end{aligned}$$

so the Hamiltonian is conserved if it does not explicitly depend on time.

Example 1: As a simple example, consider the 2-dimensional Kepler problem, with Lagrangian

$$L = \frac{1}{2}m\left(\dot{r}^2 + r^2\dot{\theta}^2\right) + \frac{GM}{r}$$

with θ cyclic. The momenta are easily seen to be

$$\begin{aligned}
p_r &= m\dot{r} \\
p_\theta &= mr^2\dot{\theta}
\end{aligned}$$

so the Hamiltonian is

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} - \frac{GM}{r}$$

Here θ is cyclic so the conserved momentum p_θ is constant. The Hamiltonian is therefore a function only of (r, p_r), with p_θ constant,

$$H\left(r, \theta, p_r, p_\theta\right) \Rightarrow H\left(r, p_r; p_\theta\right)$$

Example 2: Let a mass, m, free to move in one direction, experience a Hooke's law restoring force, $F = -kx$. Solve Hamilton's equations and study the motion of system in phase space. The Lagrangian for this system is

$$\begin{aligned}
L &= T - V \\
&= \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2
\end{aligned}$$

The conjugate momentum is just

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

so the Hamiltonian is

$$\begin{aligned} H &= p\dot{x} - L \\ &= \frac{p^2}{m} - \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 \\ &= \frac{p^2}{2m} + \frac{1}{2}kx^2 \\ &= \frac{1}{2m}\left(p^2 + m^2\omega^2x^2\right) \end{aligned}$$

We may write this in terms of $\xi^A = (x, p)$ as

$$H = \frac{1}{2m}H_{AB}\xi^A\xi^B$$

where

$$H_{AB} = \begin{pmatrix} 1 & 0 \\ 0 & m^2\omega^2 \end{pmatrix}$$

Since $\frac{\partial H}{\partial t} = 0$, $E = H$ is a constant of the motion. We see immediately that the solution is an ellipse in phase space, $E = \frac{1}{2m}\left(p^2 + m^2\omega^2x^2\right)$, or

$$\frac{1}{2mE}p^2 + \frac{m\omega^2}{2E}x^2 = 1$$

The solution with initial conditions $x(0) = x_0, p(0) = p_0$ has $E = \frac{1}{2m}\left(p_0^2 + m^2\omega^2x_0^2\right)$

$$\begin{aligned} x &= \sqrt{\frac{2mE}{m^2\omega^2}}\sin\lambda \\ p &= \sqrt{2mE}\cos\lambda \end{aligned}$$

where λ is some function of time. To find λ, we look at one of Hamilton's equations,

$$\begin{aligned} \dot{x} &= \frac{\partial H}{\partial p} \\ &= \frac{p}{m} \\ \sqrt{\frac{2mE}{m^2\omega^2}}\dot{\lambda}\cos\lambda &= \frac{\sqrt{2mE}}{m}\cos\lambda \\ \dot{\lambda} &= \omega \\ \lambda &= \omega t + \varphi_0 \end{aligned}$$

and therefore

$$\begin{aligned} x &= \sqrt{\frac{2mE}{m^2\omega^2}}\sin(\omega t + \varphi_0) \\ p &= \sqrt{2mE}\cos(\omega t + \varphi_0) \end{aligned}$$

where $\sqrt{\frac{2mE}{m^2\omega^2}}\cos\varphi_0 = x_0$ and $p_0 = \sqrt{2mE}\sin\varphi_0$, or,

$$\begin{aligned} \cos\varphi_0 &= \frac{m\omega x_0}{\sqrt{2mE}} \\ \sin\varphi_0 &= \frac{p_0}{\sqrt{2mE}} \end{aligned}$$

4 The symplectic form

4.1 Writing Hamilton's equations with unified variables

In order to fully appreciate the power and uses of Hamiltonian mechanics, we develop some formal properties. First, we write Hamilton's equations,

$$\begin{aligned} \dot{x}_k &= \frac{\partial H}{\partial p_k} \\ \dot{p}_k &= -\frac{\partial H}{\partial x_k} \end{aligned}$$

for $k = 1, \ldots, n$, in a different way. Define a unified name for our $2n$ coordinates,

$$\xi_A = (x_i, p_j)$$

for $A = 1, \ldots, 2n$. That is, more explicitly, for $i = 1, \ldots, n$,

$$\begin{aligned} \xi_i &= x_i \\ \xi_{n+i} &= p_i \end{aligned}$$

We may immediately write the left side of both of Hamilton's equations at once as

$$\dot{\xi}_A = (\dot{x}_i, \dot{p}_j)$$

The right side of the equations involves all of the partial derivatives of the Hamiltonian,

$$\frac{\partial H}{\partial \xi_A} = \left(\frac{\partial H}{\partial x_i}, \frac{\partial H}{\partial p_j} \right)$$

but there is a difference of a minus sign between the two equations and the interchange of x_i and p_i. We incorporate this by introducing a matrix called the *symplectic form*,

$$\Omega_{AB} = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix} \tag{8}$$

where $[\mathbf{1}]_{ij} = \delta_{ij}$ is the $n \times n$ identity matrix. Then, using the summation convention, Hamilton's equations, Eqs.(5) amd (6), take the form of a single expression,

$$\dot{\xi}_A = \Omega_{AB} \frac{\partial H}{\partial \xi_B} \tag{9}$$

We may check this by writing it out explicitly,

$$\begin{aligned} \begin{pmatrix} \dot{x}_i \\ \dot{p}_j \end{pmatrix} &= \begin{pmatrix} 0 & \delta_{ik} \\ -\delta_{jm} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial H}{\partial x_m} \\ \frac{\partial H}{\partial p_k} \end{pmatrix} \\ &= \begin{pmatrix} \delta_{ik} \frac{\partial H}{\partial p_k} \\ -\delta_{jm} \frac{\partial H}{\partial x_m} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial H}{\partial p_i} \\ -\frac{\partial H}{\partial x_j} \end{pmatrix} \end{aligned}$$

Example: Coupled pendula For the example of two simple pendula coupled by a spring, we found the Hamiltonian for small angles to be Eq.(7),

$$H = \frac{1}{2ml^2}\left(p_1^2+p_2^2\right)+\frac{1}{2}kl^2\left(\theta_1-\theta_2\right)^2+\frac{1}{2}mgl\left(\theta_1^2+\theta_2^2\right)$$

and we set $\xi_1=\theta_1, \xi_2=\theta_2, \xi_3=p_1$ and $\xi_4=p_2$. In terms of these, the Hamiltonian may be written as a symmetric quadratic form

$$\begin{aligned} H &= \frac{1}{2}H_{AB}\xi_A\xi_B \\ H_{AB} &= \begin{pmatrix} kl^2+mgl & -kl^2 & 0 & 0 \\ -kl^2 & kl^2+mgl & 0 & 0 \\ 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \end{pmatrix} \end{aligned}$$

with derivative,

$$\frac{\partial}{\partial\xi_C}H = \frac{1}{2}H_{AB}\delta_{AC}\xi_B+\frac{1}{2}H_{AB}\xi_A\delta_{BC} = H_{CB}\xi_B$$

Hamilton's equations are then $\dot{\xi}_A = \Omega_{AB}H_{BC}\xi_C$. Expanding this in matrices and multiplying them out,

$$\begin{aligned} \begin{pmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \\ \dot{\xi}_3 \\ \dot{\xi}_4 \end{pmatrix} &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} kl^2+mgl & -kl^2 & 0 & 0 \\ -kl^2 & kl^2+mgl & 0 & 0 \\ 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \\ -kl^2-mgl & kl^2 & 0 & 0 \\ kl^2 & -kl^2-mgl & 0 & 0 \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{ml^2}\xi_3 \\ \frac{1}{ml^2}\xi_4 \\ -kl^2\xi_1-mgl\xi_1+kl^2\xi_2 \\ -kl^2\xi_2-mgl\xi_2+kl^2\xi_1 \end{pmatrix} \end{aligned}$$

so that we recover

$$\begin{pmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \\ \dot{\xi}_3 \\ \dot{\xi}_4 \end{pmatrix} = \begin{pmatrix} \frac{1}{ml^2}\xi_3 \\ \frac{1}{ml^2}\xi_4 \\ -kl^2\left(\xi_1-\xi_2\right)-mgl\xi_1 \\ kl^2\left(\xi_1-\xi_2\right)-mgl\xi_2 \end{pmatrix}$$

as expected.

4.1.1 Diagonalizing the Hamiltonian

One systematic method of solution is to diagonalize the Hamiltonian. With

$$H_{AB} = \begin{pmatrix} kl^2+mgl & -kl^2 & 0 & 0 \\ -kl^2 & kl^2+mgl & 0 & 0 \\ 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \end{pmatrix}$$

we see that we only need to diagonalize the upper left quadrant,

$$H_{ij} = \begin{pmatrix} kl^2+mgl & -kl^2 \\ -kl^2 & kl^2+mgl \end{pmatrix}$$

This has the form

$$H = \begin{pmatrix} a & b \\ b & a \end{pmatrix}$$

The eigenvalues are found by solving

$$\begin{aligned} 0 &= \det\left(H_{ij} - \lambda\delta_{ij}\right) \\ &= (a-\lambda)^2 - b^2 \\ a - \lambda &= \pm b \\ \lambda &= a \pm b \end{aligned}$$

and the eigenvectors satisfy

$$\begin{pmatrix} a & b \\ b & a \end{pmatrix}\begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix} = (a \pm b)\begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix}$$

so for the + sign we need

$$\begin{aligned} au_+ + bv_+ &= (a+b)\,u_+ \\ bu_+ + av_+ &= (a+b)\,v_+ \end{aligned}$$

Solving, we see that $v_+ = u_+$. For the $-$ sign, we need $v_- = -u_-$. Forming a matrix of the normalized eigvectors,

$$O = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

we diagonalize with a similarity transformation,

$$\begin{aligned} O^t H O &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a & b \\ b & a \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} a-b & a+b \\ b-a & a+b \end{pmatrix} \\ &= \frac{1}{2}\begin{pmatrix} 2\,(a-b) & 0 \\ 0 & 2\,(a+b) \end{pmatrix} \\ &= \begin{pmatrix} a-b & 0 \\ 0 & a+b \end{pmatrix} \end{aligned}$$

Writing the four dimensional version of the transformation as $O = \begin{pmatrix} O & 0 \\ 0 & 1 \end{pmatrix}$ and performing the same transformation on Hamilton's equation,

$$\begin{aligned} O^t\dot{\xi} &= O^t\Omega O O^t H O O^t \xi \\ O^t\dot{\xi}_A &= O^t\Omega O\begin{pmatrix} a-b & 0 & 0 & 0 \\ 0 & a+b & 0 & 0 \\ 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \end{pmatrix} \\ \begin{pmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \\ \dot{\xi}_3 \\ \dot{\xi}_4 \end{pmatrix} &= \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} kl^2 + mgl & -kl^2 & 0 & 0 \\ -kl^2 & kl^2 + mgl & 0 & 0 \\ 0 & 0 & \frac{1}{ml^2} & 0 \\ 0 & 0 & 0 & \frac{1}{ml^2} \end{pmatrix}\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \\ \xi_4 \end{pmatrix} \end{aligned}$$

We also need

$$
\begin{aligned}
O^t\Omega O &= \begin{pmatrix} O^t & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} O & 0 \\ 0 & 1 \end{pmatrix} \\
&= \begin{pmatrix} O^t & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -O & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & O^t \\ -O & 0 \end{pmatrix}
\end{aligned}
$$

$$
\begin{aligned}
O^t\Omega O &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 & & \\ 1 & 1 & & \\ & & \sqrt{2} & \\ & & & \sqrt{2} \end{pmatrix}\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & & \\ -1 & 1 & & \\ & & \sqrt{2} & \\ & & & \sqrt{2} \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 1 & -1 & & \\ 1 & 1 & & \\ & & \sqrt{2} & \\ & & & \sqrt{2} \end{pmatrix}\begin{pmatrix} 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 0 & 0 & \sqrt{2} & -\sqrt{2} \\ 0 & 0 & \sqrt{2} & \sqrt{2} \\ -\sqrt{2} & & & \\ & -\sqrt{2} & & \end{pmatrix}
\end{aligned}
$$

We do this by first finding the eigenvalues and eigenvectors. The eigenvalues satisfy

$$
\begin{aligned}
\det\left(H_{ij} - \lambda\delta_{ij}\right) &= 0 \\
0 &= \det\begin{pmatrix} kl^2 + mgl - \lambda & -kl^2 \\ -kl^2 & kl^2 + mgl - \lambda \end{pmatrix} \\
&= \left(kl^2 + mgl - \lambda\right)\left(kl^2 + mgl - \lambda\right) - k^2l^4 \\
&= \left(kl^2 + mgl\right)^2 - 2\lambda\left(kl^2 + mgl\right) + \lambda^2 - k^2l^4
\end{aligned}
$$

Solving the quadratic,

$$
\begin{aligned}
&= \left(kl^2 + mgl\right)^2 - 2\lambda\left(kl^2 + mgl\right) + \lambda^2 - k^2l^4 \\
\lambda &= \frac{1}{2}\left(2\left(kl^2 + mgl\right) \pm \sqrt{4\left(kl^2 + mgl\right)^2 + 4k^2l^4}\right) \\
&= kl^2 + mgl \pm \sqrt{2mgl^3k + m^2g^2l^2 + 2k^2l^4}
\end{aligned}
$$

4.2 Properties of the symplectic form

We note a number of important properties of the symplectic form. First, it is antisymmetric,

$$
\begin{aligned}
\Omega^t &= -\Omega \\
\Omega_{AB} &= -\Omega_{BA}
\end{aligned}
$$

and it squares to minus the $2n$-dimensional identity,

$$
\Omega^2 = -\mathbf{1}
$$

$$\begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}\begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix} = \begin{pmatrix} -\mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$
$$= -\begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix}$$

We also have

$$\Omega^t = \Omega^{-1}$$

since $\Omega^t = -\Omega$, and therefore $\Omega\Omega^t = \Omega(-\Omega) = -\Omega^2 = \mathbf{1}$. Since all components of Ω_{AB} are constant, it is also true that

$$\partial_A \Omega_{BC} = \frac{\partial}{\partial \xi_A}\Omega_{BC} = 0$$

This last condition does not hold in every basis, however.

The defining properties of the symplectic form, necessary and sufficient to guarantee that it has the properties we require for Hamiltonian mechanics are that it be a $2n \times 2n$ matrix satisfying two properties at each point of phase space:

1. $\Omega^2 = -\mathbf{1}$
2. $\partial_A \Omega_{BC} + \partial_B \Omega_{CA} + \partial_C \Omega_{AB} = 0$

The first of these is enough for there to exist a change of basis so that $\Omega_{AB} = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}$ at any given point, while the vanishing combination of derivatives insures that this may be done at *every* point of phase space.

4.3 Change of coordinates

Consider what happens to Hamilton's equations if we want to change to a new set of phase space coordinates, $\chi^A = \chi^A(\xi)$. Let the inverse transformation be $\xi^A(\chi)$. The time derivatives become

$$\frac{d\xi^A}{dt} = \frac{\partial \xi^A}{\partial \chi^B}\frac{d\chi^B}{dt}$$

while the right side of Hamilton's equation becomes

$$\Omega^{AB}\frac{\partial H}{\partial \xi^B} = \Omega^{AB}\frac{\partial \chi^C}{\partial \xi^B}\frac{\partial H}{\partial \chi^C}$$

Equating these expressions,

$$\frac{\partial \xi^A}{\partial \chi^B}\frac{d\chi^B}{dt} = \Omega^{AB}\frac{\partial \chi^D}{\partial \xi^B}\frac{\partial H}{\partial \chi^D}$$

Noticing that the inverse to the Jacobian matrix $\frac{\partial \xi^A}{\partial \chi^B}$ is just $\frac{\partial \chi^A}{\partial \xi^B}$,

$$\frac{\partial \chi^A}{\partial \xi^C}\frac{\partial \xi^C}{\partial \chi^B} = \delta^A_B$$

we multiply by $\frac{\partial \chi^C}{\partial \xi^A}$ to get

$$\begin{aligned} \frac{\partial \chi^C}{\partial \xi^A}\frac{\partial \xi^A}{\partial \chi^B}\frac{d\chi^B}{dt} &= \frac{\partial \chi^C}{\partial \xi^A}\Omega^{AB}\frac{\partial \chi^D}{\partial \xi^B}\frac{\partial H}{\partial \chi^D} \\ \delta^C_B \frac{d\chi^B}{dt} &= \frac{\partial \chi^C}{\partial \xi^A}\Omega^{AB}\frac{\partial \chi^D}{\partial \xi^B}\frac{\partial H}{\partial \chi^D} \end{aligned}$$

and finally

$$\frac{d\chi^C}{dt} = \left(\frac{\partial\chi^C}{\partial\xi^A}\Omega^{AB}\frac{\partial\chi^D}{\partial\xi^B}\right)\frac{\partial H}{\partial\chi^D}$$

Defining the symplectic form in the new coordinate system,

$$\tilde{\Omega}^{CD} \equiv \frac{\partial\chi^C}{\partial\xi^A}\Omega^{AB}\frac{\partial\chi^D}{\partial\xi^B}$$

we see that Hamilton's equations are entirely the same if the transformation leaves the symplectic form invariant,

$$\tilde{\Omega}^{CD} = \Omega^{CD}$$

Any linear transformation $M^A{}_B$ leaving the symplectic form invariant,

$$\Omega^{AB} \equiv M^A{}_C M^B{}_D \Omega^{CD}$$

is called a symplectic transformation. Coordinate transformations which are symplectic transformations at each point are called *canonical.* Therefore those functions $\chi^A(\xi)$ satisfying

$$\Omega^{CD} \equiv \frac{\partial\chi^C}{\partial\xi^A}\Omega^{AB}\frac{\partial\chi^D}{\partial\xi^B}$$

are canonical transformations. Canonical transformations preserve Hamilton's equations.

4.4 Poincaré sections

The phase space description of classical systems are equivalent to the configuration space solutions and are often easier to interpret because more information is displayed at once. The price we pay for this is the doubled dimension – paths rapidly become difficult to plot. To offset this problem, we can use *Poincaré sections* – projections of the phase space plot onto subspaces that cut across the trajectories. Sometimes the patterns that occur on Poincaré sections show that the motion is confined to specific regions of phase space, even when the motion never repeats itself. These techniques allow us to study systems that are *chaotic*, meaning that the phase space paths through nearby points diverge rapidly. See the Wikipedia page on Chaos Theory. For more detail, read Gleick, Chaos: Making a New Science.

5 Poisson brackets

We may also write Hamilton's equations in terms of Poisson brackets between *dynamical variables.* By a dynamical variable, we mean any function $f = f\left(\xi^A\right)$ of the canonical coordinates used to describe a physical system.

We define the Poisson bracket of any two dynamical variables f and g by

$$\begin{aligned} \{f, g\}_\xi &= \Omega^{AB}\frac{\partial f}{\partial\xi^A}\frac{\partial g}{\partial\xi^B} \\ &= \frac{\partial f}{\partial x^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x^i} \end{aligned} \tag{10}$$

The importance of this product is that it is preserved by canonical transformations. We see this as follows.

Let ξ^A be any set of phase space coordinates in which Hamilton's equations take the form given in Eq.(9), $\frac{d\xi^A}{dt} = \Omega^{AB}\frac{\partial H}{\partial\xi^B}$, and let f and g be any two dynamical variables. Denote the Poisson bracket of f and g in the coordinates ξ^A be denoted by $\{f,g\}_\xi$. In a different set of coordinates, $\chi^A(\xi)$, we have

$$\begin{aligned}
\{f,g\}_\chi &= \Omega^{AB}\frac{\partial f}{\partial\chi^A}\frac{\partial g}{\partial\chi^B} \\
&= \Omega^{AB}\left(\frac{\partial\xi^C}{\partial\chi^A}\frac{\partial f}{\partial\xi^C}\right)\left(\frac{\partial\xi^D}{\partial\chi^B}\frac{\partial g}{\partial\xi^D}\right) \\
&= \left(\frac{\partial\xi^C}{\partial\chi^A}\Omega^{AB}\frac{\partial\xi^D}{\partial\chi^B}\right)\frac{\partial f}{\partial\xi^C}\frac{\partial g}{\partial\xi^D}
\end{aligned}$$

Therefore, if the coordinate transformation is canonical, we have

$$\frac{\partial\xi^C}{\partial\chi^A}\Omega^{AB}\frac{\partial\xi^D}{\partial\chi^B} = \Omega^{CD}$$

and therefore,

$$\{f,g\}_\chi = \Omega^{AB}\frac{\partial f}{\partial\xi^C}\frac{\partial g}{\partial\xi^D} = \{f,g\}_\xi$$

and the Poisson bracket is unchanged. We conclude that canonical transformations preserve all Poisson brackets.

Conversely, a transformation which preserves all Poisson brackets satisfies

$$\begin{aligned}
\{f,g\}_\chi &= \{f,g\}_\xi \\
\left(\frac{\partial\xi^C}{\partial\chi^A}\Omega^{AB}\frac{\partial\xi^D}{\partial\chi^B}\right)\frac{\partial f}{\partial\xi^C}\frac{\partial g}{\partial\xi^D} &= \Omega^{CD}\frac{\partial f}{\partial\xi^C}\frac{\partial g}{\partial\xi^D}
\end{aligned}$$

for all f,g and must therefore be canonical.

An important special case of the Poisson bracket occurs when one of the functions is the Hamiltonian. In that case, we have

$$\begin{aligned}
\{f,H\} &= \Omega^{AB}\frac{\partial f}{\partial\xi^A}\frac{\partial H}{\partial\xi^B} \\
&= \frac{\partial f}{\partial x^i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p^i}\frac{\partial H}{\partial x_i} \\
&= \frac{\partial f}{\partial x^i}\frac{dx^i}{dt} - \frac{\partial f}{\partial p^i}\left(-\frac{dp_i}{dt}\right) \\
&= \frac{df}{\partial t} - \frac{\partial f}{\partial t}
\end{aligned}$$

or simply,

$$\frac{df}{\partial t} = \{f,H\} + \frac{\partial f}{\partial t}$$

This shows that as the system evolves classically, the total time rate of change of any dynamical variable is the sum of the Poisson bracket with the Hamiltonian and the partial time derivative. If a dynamical variable has no explicit time dependence, $\frac{\partial f}{\partial t} = 0$, then the total time derivative is just the Poisson bracket with the Hamiltonian. In particular, for the Hamiltonian itself.

$$\begin{aligned}
\frac{dH}{dt} &= \{H,H\} + \frac{\partial H}{\partial t} \\
&= \frac{\partial H}{\partial t}
\end{aligned}$$

so if the Hamiltonian is not explicitly time-dependent, then it is the then energy, and a constant of the motion.

The coordinates provide another important special case. Since neither x^i nor p_i has any explicit time dependence, we have

$$
\begin{aligned}
\frac{dx^i}{dt} &= \left\{H, x^i\right\} \\
\frac{dp_i}{dt} &= \{H, p_i\}
\end{aligned}
$$

or simply

$$
\dot{\xi}^A = \left\{H, \xi^A\right\} \tag{11}
$$

We check directly that this reproduces Hamilton's equations,

$$
\begin{aligned}
\frac{dq_i}{dt} &= \left\{H, x^i\right\} \\
&= \sum_{j=1}^{N} \left(\frac{\partial x^i}{\partial x^j}\frac{\partial H}{\partial p_j} - \cancelto{0}{\frac{\partial x^i}{\partial p_j}}\frac{\partial H}{\partial x^j} \right) \\
&= \sum_{j=1}^{N} \delta_{ij}\frac{\partial H}{\partial p_j} \\
&= \frac{\partial H}{\partial p_i}
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{dp_i}{dt} &= \{H, p_i\} \\
&= \sum_{j=1}^{N} \left(\cancelto{0}{\frac{\partial p_i}{\partial q_j}}\frac{\partial H}{\partial p_j} - \frac{\partial p_i}{\partial p_j}\frac{\partial H}{\partial q_j} \right) \\
&= -\frac{\partial H}{\partial q_i}
\end{aligned}
$$

where we use the fact that, since q_i, p_i and are all independent and do not depend explicitly on time, $\frac{\partial q_i}{\partial p_j} = \frac{\partial p_i}{\partial q_j} = 0 = \frac{\partial q_i}{\partial t} = \frac{\partial p_i}{\partial t}$.

More generally, any dynamical variable with no explicit time dependence, $\frac{\partial f}{\partial t} = 0$, is a constant of the motion if and only if it has vanishing Poisson bracket with the Hamiltonian, $\{H, f\} = 0$.

6 Canonical transformations

We now define the *fundamental Poisson brackets*. Suppose x^i and p_j are a set of coordinates on phase space such that Hamilton's equations hold. Since they themselves are functions of (x^m, p_n) they are dynamical variables and we may compute their Poisson brackets with one another,

$$
\begin{aligned}
\left\{x^i, x^j\right\}_{\xi} &= \Omega^{AB}\frac{\partial x^i}{\partial \xi^A}\frac{\partial x^j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial x^i}{\partial x^m}\frac{\partial x^j}{\partial p_m} - \frac{\partial x^i}{\partial p_m}\frac{\partial x^j}{\partial x^m} \right) \\
&= 0
\end{aligned}
$$

for x^i with x^j,

$$\begin{aligned}
\left\{x^i, p_j\right\}_\xi = -\left\{p_j, x^i\right\}_\xi &= \Omega^{AB} \frac{\partial x^i}{\partial \xi^A} \frac{\partial p_j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial x^i}{\partial x^m} \frac{\partial p_j}{\partial p_m} - \frac{\partial x^i}{\partial p_m} \frac{\partial p_j}{\partial x^m} \right) \\
&= \sum_{m=1}^{N} \delta^i_m \delta^m_j \\
&= \delta^i_j
\end{aligned}$$

for x^i with p_j and finally

$$\begin{aligned}
\left\{p_i, p_j\right\}_\xi &= \Omega^{AB} \frac{\partial p_i}{\partial \xi^A} \frac{\partial p_j}{\partial \xi^B} \\
&= \sum_{m=1}^{N} \left(\frac{\partial p_i}{\partial x^m} \frac{\partial p_j}{\partial p_m} - \frac{\partial p_i}{\partial p_m} \frac{\partial p_j}{\partial x^m} \right) \\
&= 0
\end{aligned}$$

for p_i with p_j. The subscript ξ on the bracket indicates that the partial derivatives are taken with respect to the coordinates $\xi^A = \left(x^i, p_j\right)$. More succinctly, we have

$$\begin{aligned}
\left\{\xi^A, \xi^B\right\}_\xi &= \Omega^{CD} \frac{\partial \xi^A}{\partial \xi^C} \frac{\partial \xi^B}{\partial \xi^D} \\
&= \Omega^{AB}
\end{aligned}$$

However, since Poisson brackets are preserved by canonical transformations, this will hold when computed with respect to any canonical coordinates, $\left\{\xi^A, \xi^B\right\}_\chi = \Omega^{AB}$. This relation is reciprocol,

$$\begin{aligned}
\left\{\chi^A, \chi^B\right\}_\xi &= \Omega^{CD} \frac{\partial \chi^A}{\partial \xi^C} \frac{\partial \chi^B}{\partial \xi^D} \\
&= \Omega^{AB}
\end{aligned}$$

so that any set of coordinates in which Hamilton's equations hold will satisfy fundamental commutation relations, and this is true regardless of the canonical coordinates used to compute the bracket.

Conversely, suppose a set of coordinates ζ^A satisfies the fundamental commutation relations,

$$\left\{\zeta^A, \zeta^B\right\}_\xi = \Omega^{AB}$$

where ξ^A are canonical. Then expanding the definition of the bracket on the left,

$$\Omega^{CD} \frac{\partial \zeta^A}{\partial \xi^C} \frac{\partial \zeta^B}{\partial \xi^D} = \Omega^{AB}$$

and the ζ^A must also be canonical.

In summary, let ξ^A be canonical. Then each of the following statements is equivalent:

1. $\chi^A(\xi)$ is a canonical transformation.
2. $\chi^A(\xi)$ is a coordinate transformation of phase space that preserves Hamilton's equations.

3. $\chi^A(\xi)$ preserves the symplectic form, according to

$$\Omega^{AB}\frac{\partial\chi^C}{\partial\xi^A}\frac{\partial\chi^D}{\partial\xi^B} = \Omega^{CD}$$

4. $\chi^A(\xi)$ satisfies the fundamental bracket relations

$$\left\{\chi^A, \chi^B\right\}_\xi = \Omega^{AB}$$

These bracket relations represent a set of integrability conditions that must be satisfied by any new set of canonical coordinates. When we formulate the problem of canonical transformations in these terms, it is not obvious what functions $q^i\left(x^j, p_j\right)$ and $\pi_i\left(x^j, p_j\right)$ will be allowed. Fortunately there is a simple procedure for generating canonical transformations, which we develop in the next section.

We end this section with three examples of canonical transformations, and one example of a non-canonical transformation.

6.1 Example: Coordinate transformations

Let $\left(x^i, p_j\right)$ be one set of canonical variables. Suppose we define new configuration space variables, q^i, be an arbitrary invertible function of the spatial coordinates:

$$q^i = q^i\left(x^j\right)$$

We seek a set of momentum variables π_j such that $\left(q^i, \pi_j\right)$ are canonical. For this they must satisfy the fundamental Poisson bracket relations:

$$\begin{aligned}
\left\{q^i, q^j\right\}_{x,p} &= 0 \\
\left\{q^i, \pi_j\right\}_{x,p} &= \delta^i_j \\
\left\{\pi_i, \pi_j\right\}_{x,p} &= 0
\end{aligned}$$

Check each:

$$\begin{aligned}
\left\{q^i, q^j\right\}_{x,p} &= \sum_{m=1}^{N}\left(\frac{\partial q^i}{\partial x^m}\frac{\partial q^j}{\partial p_m} - \frac{\partial q^i}{\partial p_m}\frac{\partial q^j}{\partial x^m}\right) \\
&= 0
\end{aligned}$$

since $\frac{\partial q^j}{\partial p_m} = 0$. For the second bracket, we require

$$\begin{aligned}
\delta^i_j &= \left\{q^i, \pi_j\right\}_{x,p} \\
&= \sum_{m=1}^{N}\left(\frac{\partial q^i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m} - \frac{\partial q^i}{\partial p_m}\frac{\partial \pi_j}{\partial x^m}\right) \\
&= \sum_{m=1}^{N}\frac{\partial q^i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m}
\end{aligned}$$

Since q^i is independent of p_m, we can satisfy this only if

$$\frac{\partial \pi_j}{\partial p_m} = \frac{\partial x^m}{\partial q^j}$$

Integrating gives

$$\pi_j = \frac{\partial x^n}{\partial q^j}p_n + c_j(x)$$

with the c_j an arbitrary functions of x^i. Choosing $c_j = 0$, we compute the final bracket:

$$\begin{aligned}
\{\pi_i, \pi_j\}_{x,p} &= \frac{\partial \pi_i}{\partial x^m}\frac{\partial \pi_j}{\partial p_m} - \frac{\partial \pi_i}{\partial p_m}\frac{\partial \pi_j}{\partial x^m} \\
&= \frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^i}p_n\right)\frac{\partial}{\partial p_m}\left(\frac{\partial x^s}{\partial q^j}p_s\right) - \frac{\partial}{\partial p_m}\left(\frac{\partial x^n}{\partial q^i}p_n\right)\frac{\partial}{\partial x^m}\left(\frac{\partial x^s}{\partial q^j}p_s\right) \\
&= \frac{\partial x^m}{\partial q^j}\frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^i}\right)p_n - \frac{\partial x^m}{\partial q^i}\frac{\partial}{\partial x^m}\left(\frac{\partial x^n}{\partial q^j}\right)p_n \\
&= \left(\frac{\partial x^m}{\partial q^j}\frac{\partial}{\partial x^m}\right)\left(\frac{\partial x^n}{\partial q^i}\right)p_n - \left(\frac{\partial x^m}{\partial q^i}\frac{\partial}{\partial x^m}\right)\left(\frac{\partial x^n}{\partial q^j}\right)p_n \\
&= \left(\frac{\partial^2 x^n}{\partial q^j \partial q^i} - \frac{\partial^2 x^n}{\partial q^i \partial q^j}\right)p_n \\
&= 0
\end{aligned}$$

Exercise: Show that the final bracket, $\{\pi_i, \pi_j\}_{x,p}$ still vanishes provided $c_i = \frac{\partial f}{\partial q^i}$ for some function $f(q)$.

Therefore, the transformations

$$\begin{aligned}
q^j &= q^j(x^i) \\
\pi_j &= \frac{\partial x^n}{\partial q^j}p_n + \frac{\partial f}{\partial q^j}
\end{aligned}$$

is a canonical transformation for any functions $q^i(x)$. This means that the symmetry group of Hamilton's equations includes the symmetry group of the Euler-Lagrange equations, and sill has some freedom.

6.2 Example 2: Interchange of x and p.

The transformation

$$\begin{aligned}
q^i &= p_i \\
\pi_i &= -x^i
\end{aligned}$$

is canonical. We easily check the fundamental brackets:

$$\begin{aligned}
\left\{q^i, q^j\right\}_{x,p} &= \{p_i, p_j\}_{x,p} = 0 \\
\left\{q^i, \pi_j\right\}_{x,p} &= \left\{p_i, -x^j\right\}_{x,p} \\
&= \left\{x^j, p_i\right\}_{x,p} \\
&= \delta^j_i \\
\{\pi_i, \pi_j\}_{x,p} &= \left\{-x^i, -x^j\right\}_{x,p} = 0
\end{aligned}$$

Interchange of x^i and p_j, with a sign, is therefore canonical. The use of generalized coordinates in Lagrangian mechanics does not include such a possibility, so again we see that Hamiltonian dynamics has a larger symmetry group than Lagrangian dynamics.

For our next example, we first show that the composition of two canonical transformations is also canonical. Let $\psi(\chi)$ and $\chi(\xi)$ both be canonical. Defining the composition transformation, $\psi(\xi) = \psi(\chi(\xi))$, we compute

$$\Omega^{CD}\frac{\partial \psi^A}{\partial \xi^C}\frac{\partial \psi^B}{\partial \xi^D} = \Omega^{CD}\left(\frac{\partial \psi^A}{\partial \chi^E}\frac{\partial \chi^E}{\partial \xi^C}\right)\left(\frac{\partial \psi^B}{\partial \chi^F}\frac{\partial \chi^F}{\partial \xi^D}\right)$$

$$
\begin{aligned}
&= \left(\frac{\partial \chi^E}{\partial \xi^C} \frac{\partial \chi^F}{\partial \xi^D} \Omega^{CD} \right) \frac{\partial \psi^A}{\partial \chi^E} \frac{\partial \psi^B}{\partial \chi^F} \\
&= \Omega^{EF} \left(\frac{\partial \psi^A}{\partial \chi^E} \right) \left(\frac{\partial \psi^B}{\partial \chi^F} \right) \\
&= \Omega^{AB}
\end{aligned}
$$

so that $\psi(\xi)$ is canonical.

6.3 Example 3: Momentum transformations

By the preceding result, the composition of an arbitratry coordinate change with x, p interchanges is canonical. Consider the effect of composing (a) an interchange, (b) a coordinate transformation, and (c) an interchange.

For (a), let

$$
\begin{aligned}
\tilde{q}^i &= p_i \\
\tilde{\pi}_i &= -x^i
\end{aligned}
$$

Then for (b) we choose an arbitrary function of $\tilde{q}^i$:

$$
\begin{aligned}
Q^i &= F^i\left(\tilde{q}^j\right) \\
P_i &= \frac{\partial \tilde{q}^n}{\partial Q^i} \tilde{\pi}_n
\end{aligned}
$$

Finally, for (c), another interchange:

$$
\begin{aligned}
q^i &= P_i \\
\pi_i &= -Q^i
\end{aligned}
$$

Combining all three, we have

$$
\begin{aligned}
q^i &= P_i = \frac{\partial \tilde{q}^n}{\partial Q^i} \tilde{\pi}_n = -\frac{\partial p^n}{\partial \pi_i} x_n \\
\pi_i &= -Q^i = F^i\left(\tilde{q}^j\right) = F^i\left(p_j\right)
\end{aligned}
$$

so that π_i is replaced by an arbitrary function of the original momenta. This establishes that replacing the momenta by any independent functions of the momenta, preserves Hamilton's equations as long as we choose the proper coordinates q^i.

6.4 Example 4: A non-canonical transformation

Let $\xi^A = \left(x^i, p_i\right)$ be canonical and set

$$
\begin{aligned}
q^i &= p^2 x^i \\
\pi_i &= \pi^i(\mathbf{x}, \mathbf{p})
\end{aligned}
$$

Then

$$
\begin{aligned}
\left\{q^i, q^j\right\} &= \sum_{m=1}^{N} \left(\frac{\partial q^i}{\partial x^m} \frac{\partial q^j}{\partial p_m} - \frac{\partial q^i}{\partial p_m} \frac{\partial q^j}{\partial x^m} \right) \\
&= \sum_{m=1}^{N} \left(\delta^i_m \left(2p^m q^j + p^2 \cancel{\frac{\partial q^j}{\partial p_m}} \right) - \left(2p^m q^i + p^2 \cancel{\frac{\partial q^i}{\partial p_m}} \right) \delta^j_m \right) \\
&= 2 \sum_{m=1}^{N} \left(p^i q^j - p^j q^i \right)
\end{aligned}
$$

which is proportional to orbital angular momentum and not zero. Therefore, any transformations of this form are not canonical.

7 Generating functions

There is a systematic approach to canonical transformations using generating functions. We will give a simple example of the technique. Given a system described by a Hamiltonian $H(x^i, p_j)$, with

$$\begin{aligned} \frac{dx^i}{dt} &= \frac{\partial H}{\partial p_i} \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial x^i} \end{aligned}$$

we seek another Hamiltonian $H'(q^i, \pi_j)$ such that the equations of motion have the same form, namely

$$\begin{aligned} \frac{dq^i}{dt} &= \frac{\partial H'}{\partial \pi_i} \\ \frac{d\pi_i}{dt} &= -\frac{\partial H'}{\partial q^i} \end{aligned}$$

in the transformed variables. The principle of least action must hold for each pair:

$$\begin{aligned} S &= \int \left(p_i dx^i - H dt\right) \\ S' &= \int \left(\pi_i dq^i - H' dt\right) \end{aligned}$$

where S and S' differ by at most a constant. Correspondingly, the integrands may differ by the addition of an exact differential, $df = \frac{df}{dt}dt$, since this will integrate to a surface term and therefore will contribute at most a constand to the action.

In general we may therefore write

$$p_i dx^i - H dt = \pi_i dq^i - H' dt + df$$

and solve for the differential df

$$df = p_i dx^i - \pi_i dq^i + (H' - H)\, dt \tag{12}$$

Notice the differentials, dx^i, dq^i, dt on the right. For the differential of f to take this form, it must be a function of x^i, q^i and t only, $f = f(\mathbf{x}, \mathbf{q}, t)$. Therefore, the differential of f is

$$df = \frac{\partial f}{\partial x^i}dx^i + \frac{\partial f}{\partial q^i}dq^i + \frac{\partial f}{\partial t}dt$$

Equating the expressions for df we match up terms to require

$$p_i = \frac{\partial f}{\partial x^i} \tag{13}$$

$$\pi_i = -\frac{\partial f}{\partial q^i} \tag{14}$$

$$H' = H + \frac{\partial f}{\partial t} \tag{15}$$

Eq.(13), where f is a given function of $\mathbf{x}, \mathbf{q}$ and t, gives q^i implicitly in terms of the original variables. Inverting this to find $q^i = q^i(\mathbf{x}, \mathbf{p}, t)$, we substitute into Eq.(14) to find $\pi_i(\mathbf{x}, \mathbf{p}, t)$. Now, inverting to find the old coordinates in terms of the new,

$$x^i(\mathbf{q}, \boldsymbol{\pi}, t), \; p_i(\mathbf{q}, \boldsymbol{\pi}, t)$$

we move to the new Hamiltonian, Eq.(15), which becomes

$$H'\left(q^i, \pi_j\right) = H\left(x^i(\mathbf{q}, \boldsymbol{\pi}, t), p_l(\mathbf{q}, \boldsymbol{\pi}, t)\right) + \frac{\partial f\left(x^i(\mathbf{q}, \boldsymbol{\pi}, t), \mathbf{q}\right)}{\partial t}$$

The function f is the *generating function* of the transformation.

There are other types of generating functions. By making a Legendre transformation, we can change the independent variables. For example, setting

$$f = p_i x^i + f_2(p_i, q_i, t)$$

we have

$$\begin{aligned} p_i dx^i - H dt &= \pi_i dq^i - H' dt + df \\ &= \pi_i dq^i - H' dt + dp_i x^i + p_i dx^i + df_2(p_i, q_i, t) \\ -H dt &= \pi_i dq^i - H' dt + dp_i x^i + df_2(p_i, q_i, t) \end{aligned}$$

so that the independent variables are now (p_i, q_i), satisfying

$$\begin{aligned} x^i &= -\frac{\partial f_2}{\partial p_i} \\ \pi_i &= \frac{\partial f_2}{\partial q^i} \\ H' &= H + \frac{\partial f_2}{\partial t} \end{aligned}$$

We may also define

$$f = -\pi_i q^i + f_3\left(x^i, \pi_j, t\right)$$

so that

$$df = -\pi_i dq^i - q^i d\pi_i + \frac{\partial f_3}{\partial x^i} dx^i + \frac{\partial f_3}{\partial \pi_i} d\pi_i + \frac{\partial f_3}{\partial t} dt$$

and therefore,

$$\begin{aligned} 0 &= -p_i dx^i + H dt + \pi_i dq^i - H' dt - \pi_i dq^i - q^i d\pi_i + \frac{\partial f_3}{\partial x^i} dx^i + \frac{\partial f_3}{\partial \pi_i} d\pi_i + \frac{\partial f_3}{\partial t} dt \\ &= \left(-p_i + \frac{\partial f_3}{\partial x^i}\right) dx^i + \left(-q^i + \frac{\partial f_3}{\partial \pi_i}\right) d\pi_i + \left(H - H' + \frac{\partial f_3}{\partial t}\right) dt \end{aligned}$$

so that

$$\begin{aligned} p_i &= \frac{\partial f_3}{\partial x^i} \\ q^i &= \frac{\partial f_3}{\partial \pi_i} \\ H' &= H + \frac{\partial f_3}{\partial t} \end{aligned}$$

The final example, $f = p_i x^i - \pi_i q^i + f_4\left(p^i, \pi_j, t\right)$, is left as an exercise.

In summary, the independent variables may be taken as either of the new coordinates $\left(q^i, \pi_j\right)$ with either of the old coordinates $\left(x^i, p_j\right)$.

7.1 Example 1

Let f_2 be a general quadratic,

$$f_2\left(p_i, q^j, t\right) = \frac{1}{2}\left(a_{ij}\left(t\right) q^i q^j + b^i{}_j\left(t\right) p_i q^j + c^{ij}\left(t\right) p_i p_j\right)$$

with a_{ij} and c^{ij} symmetric. Then $f = p_i x^i + f_2$. Computing the differential of f,

$$\begin{aligned} df &= d\left(p_i x^i + f_2\right) \\ &= dp_i x^i + p_i dx^i + \frac{1}{2} d\left(a_{ij}\left(t\right) q^i q^j + b^i{}_j\left(t\right) p_i q^j + c^{ij}\left(t\right) p_i p_j\right) \\ &= x^i dp_i + p_i dx^i + \frac{1}{2}\left(\dot{a}_{ij}\left(t\right) q^i q^j + \dot{b}^i{}_j\left(t\right) p_i q^j + \dot{c}^{ij}\left(t\right) p_i p_j\right) dt \\ &\quad + \frac{1}{2}\left(2a_{ij}\left(t\right) q^i dq^j + b^i{}_j\left(t\right) dp_i q^j + b^i{}_j\left(t\right) p_i dq^j + 2c^{ij}\left(t\right) p_i dp_j\right) \end{aligned}$$

we write Eq.(12) as

$$0 = df - p_i dx^i + \pi_i dq^i - \left(H' - H\right) dt$$

and substitute,

$$\begin{aligned} 0 &= df - p_i dx^i + \pi_i dq^i - \left(H' - H\right) dt \\ &= dp_i x^i + p_i dx^i + \frac{1}{2}\left(\dot{a}_{ij}\left(t\right) q^i q^j + \dot{b}^i{}_j\left(t\right) p_i q^j + \dot{c}^{ij}\left(t\right) p_i p_j\right) dt \\ &\quad + a_{ij}\left(t\right) q^i dq^j + \frac{1}{2} b^i{}_j\left(t\right) dp_i q^j + \frac{1}{2} b^i{}_j\left(t\right) p_i dq^j + c^{ij}\left(t\right) p_i dp_j \\ &\quad - p_i dx^i + \pi_i dq^i - \left(H' - H\right) dt \end{aligned}$$

Canceling $p_i dx^i$ and collecting terms,

$$\begin{aligned} 0 &= \left(x^i + \frac{1}{2} b^i{}_j\left(t\right) q^j + c^{ji}\left(t\right) p_j\right) dp_i \\ &\quad + \left(\pi_i + a_{ji}\left(t\right) q^j + \frac{1}{2} b^j{}_i\left(t\right) p_j\right) dq^i \\ &\quad + \left(H - H' + \frac{1}{2}\left(\dot{a}_{ij}\left(t\right) q^i q^j + \dot{b}^i{}_j\left(t\right) p_i q^j + \dot{c}^{ij}\left(t\right) p_i p_j\right)\right) dt \end{aligned}$$

Therefore,

$$\begin{aligned} x^i &= -\frac{1}{2} b^i{}_j\left(t\right) q^j - c^{ji}\left(t\right) p_j \\ \pi_i &= -a_{ji}\left(t\right) q^j - \frac{1}{2} b^j{}_i\left(t\right) p_j \\ H' &= H + \frac{1}{2}\left(\dot{a}_{ij}\left(t\right) q^i q^j + \dot{b}^i{}_j\left(t\right) p_i q^j + \dot{c}^{ij}\left(t\right) p_i p_j\right) \end{aligned}$$

Solving for the new coordinate, we invert the matrix $b^i{}_j$,

$$q^m = -2\left[b^{-1}\right]^m{}_i\left(x^i + c^{ij}\left(t\right) p_j\right)$$

Then the new momentum is

$$\pi_i = 2a_{im}\left[b^{-1}\right]^m{}_i\left(x^i + c^{ij} p_j\right) - \frac{1}{2} b^j{}_i\left(t\right) p_j$$

Finally, inverting these and writing

$$H\left(x^i,p_i\right) = H\left(x^i\left(\mathbf{q},\boldsymbol{\pi}\right),p_i\left(\mathbf{q},\boldsymbol{\pi}\right)\right)$$

we have the new Hamiltonian,

$$H'\left(\mathbf{q},\boldsymbol{\pi}\right) = H\left(x^i\left(\mathbf{q},\boldsymbol{\pi}\right),p_i\left(\mathbf{q},\boldsymbol{\pi}\right)\right)+\frac{1}{2}\left(\dot{a}_{ij}\left(t\right)q^iq^j+\dot{b}^i{}_j\left(t\right)p_iq^j+\dot{c}^{ij}\left(t\right)p_ip_j\right)$$

8 Hamilton-Jacobi theory

We conclude with the crowning theorem of Hamiltonian dynamics: a proof that for any Hamiltonian dynamical system there exists a canonical transformation to a set of variables on phase space such that the paths of motion reduce to single points. Clearly, this theorem shows the power of canonical transformations! The theorem relies on describing solutions to the Hamilton-Jacobi equation, which we introduce first.

8.1 Integrability of the action

We first define Hamilton's principal function. Let $x^i\left(t\right)$ and $p_i\left(t\right)$ satisfy Hamilton's equations of motion, and ask for the integrability condition for the action. That is, we would like to know when the action is a function and not a functional, $S\left[x^i\left(t\right)\right]\Rightarrow S\left(x^i,t\right)$. The condition we need is just like the vanishing curl of a force required for the existence of a potential function. Thinking of the $n+1$ dimensional vector$P_a=\left(p_i,-H\right)$ integrated along a curve in $dX^a=\left(x^i,t\right)$-space where $a-=1,\ldots,n+1$, the action is

$$S = \int\limits_A^B p_idx^i-Hdt=\int\limits_A^B P_adX^a$$

For S to be a function, this integral must be independent of path. Consider any two paths, C_1 and C_2 from A to B. We require $\int_{C_1}P_adX^a=\int_{C_2}P_adX^a$, or combining the two paths taking one up and one down to give a closed loop, C_1-C_2,

$$\oint\limits_{C_1-C_2} P_adX^a = 0$$

Using Stokes' theorem in $n+1$ dimensions, this becomes

$$\begin{aligned} 0 &= \oint\limits_{C_1-C_2} P_adX^a \\ &= \iint\limits_S \left(\frac{\partial P_a}{\partial X^b}-\frac{\partial P_b}{\partial X^a}\right)d^2S^{ab} \end{aligned}$$

for any surface S with boundary C_1-C_2. Since S and its boundary are arbitrary, the integrand must vanish,

$$\frac{\partial P_a}{\partial X^b}-\frac{\partial P_b}{\partial X^a}=0$$

This is the integrability condition for the action.

Writing this in terms of $P_a=\left(p_i,H\right)$ and $X^b=\left(x^j,t\right)$ we find four relations,

$$\begin{aligned} \frac{\partial p_i}{\partial x^j}-\frac{\partial p_j}{\partial x^i} &= 0 \\ -\frac{\partial H}{\partial x^i}-\frac{dp_i}{dt} &= 0 \end{aligned}$$

$$
\begin{aligned}
\frac{dp_i}{dt} + \frac{\partial H}{\partial x^i} &= 0 \\
-\frac{\partial H}{\partial t} + \frac{\partial H}{\partial t} &= 0
\end{aligned}
$$

The first is satisfied because x^i and p_j are independent, $\frac{\partial p_i}{\partial x^j} = 0$, the middle two are equivalent and give one of Hamilton's equations, and the final equation is an identity. Therefore, S is a function if $\dot{p}_i = -\frac{\partial H}{\partial x^i}$.

The condition is not unique. Since we may integrate by parts,

$$
\begin{aligned}
S &= \int_A^B p_i dx^i - H dt \\
&= \int_A^B d\left(p_i x^i\right) - x^i dp_i - H dt \\
&= p_i x^i \big|_A^B - \int \left(x^i dp_i + H dt\right)
\end{aligned}
$$

a similar argument applied to $\int \left(x^i dp_i + H dt\right)$ shows that $\dot{x}^i = \frac{\partial H}{\partial p_i}$ gives integrability. Therefore, if the family of curves, $\left(x^i(t), p_j(t)\right)$ solve Hamilton's equations, then evaluating the action on those curves gives a *function.*

Exercise: Carry out the details of the demonstration that S becomes a function if $\dot{x}^i = \frac{\partial H}{\partial p_i}$

Finally, suppose one of Hamilton's equations holds, say $\dot{p}_i = -\frac{\partial H}{\partial x^i}$. Then

$$
\begin{aligned}
S\left(x^i, t\right) &= \int_A^B \left(p_i dx^i - H dt\right) \\
&= \int_A^B \left(d\left(p_i x^i\right) - x^i dp_i - H dt\right) \\
&= \left(p_i x^i\right)\big|_A^B - \int_A^B \left(x^i dp_i - H dt\right)
\end{aligned}
$$

so that

$$
\int_A^B \left(x^i dp_i - H dt\right) = \left(p_i x^i\right)\big|_A^B - S\left(x^i, t\right) = \tilde{S}\left(x^i, t\right)
$$

where $\tilde{S}\left(x^i, t\right)$ is also a function. The integrability condition for $\tilde{S}\left(x^i, t\right)$ must hold, and we have the second Hamilton equation, $\dot{x}^i = \frac{\partial H}{\partial p_i}$.

Therefore, the action is a function if and only if Hamilton's equations hold.

8.2 The Hamilton-Jacobi equation

Conversely, suppose we replace the action with a function, $S[x] \to \mathcal{S}\left(x^i, t\right)$. Then

$$
\mathcal{S}\left(x^i, t\right) = \int p_i dx^i - H dt
$$

implies

$$\begin{aligned}
d\mathcal{S} &= p_i dx^i - H dt \\
\frac{\partial \mathcal{S}}{\partial x^i} dx^i + \frac{\partial \mathcal{S}}{\partial t} dt &= p_i dx^i - H dt
\end{aligned}$$

so that

$$\begin{aligned}
p_i &= \frac{\partial \mathcal{S}}{\partial x^i} \\
H\left(x^i, p_j, t\right) &= -\frac{\partial \mathcal{S}}{\partial t}
\end{aligned}$$

If we replace p_j in the Hamiltonian, we get a differential equation for Hamilton's principal function,

$$H\left(x^i, \frac{\partial \mathcal{S}}{\partial x^j}, t\right) = -\frac{\partial \mathcal{S}}{\partial t} \tag{16}$$

This is the *Hamilton-Jacobi* equation. The function $\mathcal{S}$ satisfying the Hamilton-Jacobi equation is called *Hamilton's principal function.*

Example: Find the Hamilton-Jacobi equation for a simple harmonic oscillator Since the Hamiltonian for the oscillator is

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2$$

the Hamilton-Jacobi equation is

$$\frac{1}{2m}\left(\frac{\partial \mathcal{S}}{\partial x}\right)^2 + \frac{1}{2} k x^2 = -\frac{\partial \mathcal{S}}{\partial t}$$

Partial differential equations have free functions in their solutions. Thus, while

$$\frac{\partial^2 f}{\partial x^2} - \frac{\partial^2 f}{\partial t^2} = 0$$

has the particular solution

$$f(x, t) = ax + by + c$$

it has the much more general solution

$$f(x, y) = g_-(x + t) + g_+(x - t)$$

for *any* two functions $g_\pm$. We therefore expect arbitrary functions in the solution for $\mathcal{S}$

8.3 The principal function as generator of a canonical transformation

Suppose we find Hamilton's principal function, $\mathcal{S}\left(x^i, t\right)$. Its relationship to the momentum, $p_i = \frac{\partial \mathcal{S}}{\partial x^i}$, suggests that we may use it as a generating function for a canonical transformation, $\mathcal{S}\left(x^i, \pi_j, t\right) = \mathcal{S}\left(x^i, t\right)$. This turns out to be especially useful.

We choose a generating function with independent variables x^i, π_j, so let

$$f = -\left(q^i - q_0^i\right)\pi_i + \mathcal{S}\left(x^i, t\right)$$

Then, substituting into Eq.(12) we have

$$\begin{aligned}
df &= p_i dx^i - \pi_i dq^i + \left(H' - H\right) dt \\
-\left(q^i - q_0^i\right) d\pi_i - \pi_i dq^i + \frac{\partial \mathcal{S}}{\partial x^i} dx^i + \frac{\partial \mathcal{S}}{\partial \pi_i} d\pi_i + \frac{\partial \mathcal{S}}{\partial t} dt &= p_i dx^i - \pi_i dq^i + \left(H' - H\right) dt \\
\frac{\partial \mathcal{S}}{\partial x^i} dx^i + \frac{\partial \mathcal{S}}{\partial \pi_i} d\pi_i + \frac{\partial \mathcal{S}}{\partial t} dt &= p_i dx^i + \left(q^i - q_0^i\right) d\pi_i + \left(H' - H\right) dt
\end{aligned}$$

so that the independent variables are now $\left(x^i, \pi_i, t\right)$. Equating like terms we must satisfy

$$\begin{aligned}
p_i &= \frac{\partial \mathcal{S}}{\partial x^i} \\
q^i &= q_0^i + \frac{\partial \mathcal{S}}{\partial \pi_i} \\
H' &= H + \frac{\partial \mathcal{S}}{\partial t}
\end{aligned}$$

But we know that Hamilton's principal function $\mathcal{S}$ satisfies

$$\begin{aligned}
\frac{\partial \mathcal{S}}{\partial x^i} &= p_i \\
\frac{\partial \mathcal{S}}{\partial \pi_i} &= 0 \\
\frac{\partial \mathcal{S}}{\partial t} &= -H
\end{aligned}$$

so the first two equations are satisfied and the new Hamilton vanishes, $H' = 0$.

The principal function has generated a transformation to a set of canonical variables for which the Hamiltonian vanishes! This makes Hamilton's equations trivial:

$$\begin{aligned}
\dot{q}^i &= 0 \\
\dot{\pi}_i &= 0
\end{aligned}$$

so $\left(q^i, \pi_j\right)$ simply stay at their initial values, $\left(q_0^i, \pi_{0j}\right)$.

8.4 Examples

8.4.1 Example 1: Free particle

The simplest example is the case of a free particle, for which the Hamiltonian is

$$H = \frac{p^2}{2m}$$

and the Hamilton-Jacobi equation is

$$\frac{\partial \mathcal{S}}{\partial t} = -\frac{1}{2m}\left(\mathcal{S}'\right)^2$$

Let

$$\mathcal{S} = f(x) - Et$$

Then $f(x)$ must satisfy

$$\frac{df}{dx} = \sqrt{2mE}$$

and therefore

$$\begin{aligned}
f(x) &= \sqrt{2mE}x - c \\
&= \pi x - c
\end{aligned}$$

where c is constant and we write the integration constant E in terms of the new (constant) momentum, $E = \frac{\pi^2}{2m}$. Hamilton's principal function is therefore

$$\mathcal{S}\left(x, \pi, t\right) = \pi x - \frac{\pi^2}{2m}t - c$$

Then, for a generating function of this type we have

$$\begin{aligned}
p &= \frac{\partial \mathcal{S}}{\partial x} = \pi \\
q &= \frac{\partial \mathcal{S}}{\partial \pi} = x - \frac{\pi}{m} t \\
H' &= H + \frac{\partial \mathcal{S}}{\partial t} = H - E
\end{aligned}$$

Because $E = H$, the new Hamiltonian, H', is zero. This means that both q and π are constant. The solution for x and p follows immediately:

$$\begin{aligned}
x &= q + \frac{\pi}{m} t \\
p &= \pi
\end{aligned}$$

We see that the new canonical variables (q, π) are just the initial position and momentum of the motion, and therefore do determine the motion. The fact that knowing q and π is equivalent to knowing the full motion rests here on the fact that S generates motion along the classical path. In fact, given initial conditions (q, π), we can use Hamilton's principal function as a generating function but treat π as the *old* momentum and x as the *new* coordinate to reverse the process above and generate $x(t)$ and p.

8.4.2 Example 2: Simple harmonic oscillator

For the simple harmonic oscillator, the Hamiltonian becomes

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2$$

and the Hamilton-Jacobi equation is

$$\frac{1}{2m} \left(\frac{\partial \mathcal{S}}{\partial x} \right)^2 + \frac{1}{2} k x^2 = -\frac{\partial \mathcal{S}}{\partial t}$$

Setting $\mathcal{S} = f(x) - Et$ then

$$\begin{aligned}
\frac{1}{2m} \left(\frac{df}{dx} \right)^2 + \frac{1}{2} k x^2 &= E \\
\frac{df}{dx} &= \sqrt{2mE - mkx^2}
\end{aligned}$$

and direct integration (see examples, below) give a solution for $\mathcal{S}$,

$$\begin{aligned}
f &= \int dx \sqrt{2mE - mkx^2} \\
&= \sqrt{2mE} \int dx \sqrt{1 - \frac{k}{2E} x^2}
\end{aligned}$$

so with $\sqrt{\frac{k}{2E}} x = \sin \mu$ we have

$$\begin{aligned}
f &= \sqrt{2mE} \int \sqrt{1 - \sin^2 \mu} \sqrt{\frac{2E}{k}} \cos \mu d\mu \\
&= \frac{2E}{\omega} \int \cos^2 \mu d\mu
\end{aligned}$$

$$\begin{aligned}
&= \frac{2E}{\omega}\int \frac{1}{2}(1+\cos 2\mu)\,d\mu \\
&= \frac{E}{\omega}\left(\mu + \frac{1}{2}\sin 2\mu\right) \\
&= \frac{E}{\omega}\left(\sin^{-1}\sqrt{\frac{k}{2E}}x + \sin\left(\sin^{-1}\sqrt{\frac{k}{2E}}x\right)\cos\left(\sin^{-1}\sqrt{\frac{k}{2E}}x\right)\right) \\
&= \frac{E}{\omega}\left(\sin^{-1}\sqrt{\frac{k}{2E}}x + \sqrt{\frac{k}{2E}}x\sqrt{1-\frac{k}{2E}x^2}\right)
\end{aligned}$$

Therefore,

$$\mathcal{S} = f(x) - Et$$

as before, $f(x)$ must satisfy

$$\frac{df}{dx} = \sqrt{2m\left(E - \frac{1}{2}kx^2\right)}$$

and therefore

$$\begin{aligned}
f(x) &= \int \sqrt{2m\left(E-\frac{1}{2}kx^2\right)}dx \\
&= \int \sqrt{\pi^2 - mkx^2}dx
\end{aligned}$$

where we have set $E = \frac{\pi^2}{2m}$. Now let $\sqrt{mk}x = \pi \sin y$. The integral is immediate:

$$\begin{aligned}
f(x) &= \int \sqrt{\pi^2 - mkx^2}dx \\
&= \frac{\pi^2}{\sqrt{mk}}\int \cos^2 y dy \\
&= \frac{\pi^2}{2\sqrt{mk}}(y + \sin y \cos y)
\end{aligned}$$

Hamilton's principal function is therefore

$$\begin{aligned}
\mathcal{S}(x,\pi,t) &= \frac{\pi^2}{2\sqrt{mk}}\left(\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right) + \sqrt{mk}\frac{x}{\pi}\sqrt{1-mk\frac{x^2}{\pi^2}}\right) - \frac{\pi^2}{2m}t - c \\
&= \frac{\pi^2}{2\sqrt{mk}}\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right) + \frac{x}{2}\sqrt{\pi^2 - mkx^2} - \frac{\pi^2}{2m}t - c
\end{aligned}$$

and we may use it to generate the canonical change of variable.

This time we have for p,

$$\begin{aligned}
p &= \frac{\partial \mathcal{S}}{\partial x} \\
&= \frac{\pi}{2}\frac{1}{\sqrt{1-mk\frac{x^2}{\pi^2}}} + \frac{1}{2}\sqrt{\pi^2 - mkx^2} + \frac{x}{2}\frac{-mkx}{\sqrt{\pi^2 - mkx^2}} \\
&= \frac{1}{\sqrt{\pi^2 - mkx^2}}\left(\frac{\pi^2}{2} + \frac{1}{2}\left(\pi^2 - mkx^2\right) - \frac{mkx^2}{2}\right) \\
&= \frac{1}{\sqrt{\pi^2 - mkx^2}}\left(\pi^2 - mkx^2\right) \\
&= \sqrt{\pi^2 - mkx^2}
\end{aligned}$$

For q,

$$
\begin{aligned}
q &= \frac{\partial \mathcal{S}}{\partial \pi} \\
&= \frac{\partial}{\partial \pi}\left(\frac{\pi^2}{2\sqrt{mk}}\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right)+\frac{x}{2}\sqrt{\pi^2-mkx^2}-\frac{\pi^2}{2m}t-c\right) \\
&= \frac{\pi}{\sqrt{mk}}\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right)-\frac{x}{2}\frac{\pi}{\sqrt{\pi^2-mkx^2}}+\frac{x}{2}\frac{\pi}{\sqrt{\pi^2-mkx^2}}-\frac{\pi}{m}t \\
&= \frac{\pi}{\sqrt{mk}}\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right)-\frac{\pi}{m}t
\end{aligned}
$$

and finally $H' = H + \frac{\partial S}{\partial t} = H - E = 0$. The first equation relates p to the energy and position, the second gives the new position coordinate q, and third equation shows that the new Hamiltonian is zero. Hamilton's equations are trivial, so that π and q are constant.

Solving for π in terms of p,

$$
\begin{aligned}
p^2 &= \pi^2 - mkx^2 \\
\pi &= \sqrt{p^2 + mkx^2}
\end{aligned}
$$

The solution for q may be solved directly for $x(q,\pi)$,

$$
\begin{aligned}
q &= \frac{\pi}{\sqrt{mk}}\sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right)-\frac{\pi}{m}t \\
\frac{\sqrt{mk}}{\pi}\left(q+\frac{\pi}{m}t\right) &= \sin^{-1}\left(\sqrt{mk}\frac{x}{\pi}\right) \\
x &= \frac{\pi}{\sqrt{mk}}\sin\frac{\sqrt{mk}}{\pi}\left(q+\frac{\pi}{m}t\right)
\end{aligned}
$$

Setting $\omega = \sqrt{\frac{k}{m}}$ and $A = \frac{\pi}{m\omega}$, the initial phase is $\varphi_0 = \frac{m\omega q}{\pi}$ and the solution is

$$
x(t) = A\sin(\varphi_0 + \omega t)
$$

The new canonical coordinates therefore characterize the initial amplitude and phase of the oscillator.

8.4.3 Example 3: One dimensional particle motion

Now suppose a particle with one degree of freedom moves in a potential $U(x)$. Little is changed. The the Hamiltonian becomes

$$
H = \frac{p^2}{2m} + U
$$

and the Hamilton-Jacobi equation is

$$
\frac{\partial S}{\partial t} = -\frac{1}{2m}(S')^2 + U(x)
$$

Letting $S = f(x) - Et$ as before, $f(x)$ must satisfy

$$
\frac{df}{dx} = \sqrt{2m(E - U(x))}
$$

and therefore

$$
\begin{aligned}
f(x) &= \int \sqrt{2m(E-U(x))}dx \\
&= \int \sqrt{\pi^2 - 2mU(x)}dx
\end{aligned}
$$

where we have set $E = \frac{\pi^2}{2m}$. Hamilton's principal function is therefore

$$S(x, \pi, t) = \int \sqrt{\pi^2 - 2mU(x)}dx - \frac{\pi^2}{2m}t - c$$

and we may use it to generate the canonical change of variable.

This time we have

$$\begin{aligned} p &= \frac{\partial S}{\partial x} = \sqrt{\pi^2 - 2mU(x)} \\ q &= \frac{\partial S}{\partial \pi} = \frac{\partial}{\partial \pi}\left(\int_{x_0}^{x} \sqrt{\pi^2 - 2mU(x)}dx\right) - \frac{\pi}{m}t \\ H' &= H + \frac{\partial S}{\partial t} = H - E = 0 \end{aligned}$$

The first and third equations are as expected, while for q we may interchange the order of differentiation and integration:

$$\begin{aligned} q &= \frac{\partial}{\partial \pi}\left(\int \sqrt{\pi^2 - 2mU(x)}dx\right) - \frac{\pi}{m}t \\ &= \int \frac{\partial}{\partial \pi}\left(\sqrt{\pi^2 - 2mU(x)}\right) dx - \frac{\pi}{m}t \\ &= \int \frac{\pi dx}{\sqrt{\pi^2 - 2mU(x)}} - \frac{\pi}{m}t \\ &= \int \frac{dx}{\sqrt{1 - \frac{U(x)}{E}}} - \frac{\pi}{m}t \end{aligned}$$

To complete the problem, we need to know the potential. However, even without knowing $U(x)$ we can make sense of this result by combining the expression for q above to our previous solution to the same problem. With $\pi^2 = 2mE$, he solution for q may be written as

$$t + \sqrt{\frac{m}{2E}}q = \sqrt{\frac{m}{2E}} \int \frac{dx}{\sqrt{1 - \frac{U(x)}{E}}}$$

There, conservation of energy gives a first integral to Newton's second law,

$$\begin{aligned} E &= \frac{p^2}{2m} + U \\ &= \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 + U \end{aligned}$$

so we arrive at the familiar quadrature

$$\begin{aligned} E &= \frac{p^2}{2m} + U \\ \frac{2E}{m} &= \left(\frac{dx}{dt}\right)^2 + \frac{2}{m}U \\ \sqrt{\frac{2E}{m}\left(1 - \frac{U}{E}\right)} &= \frac{dx}{dt} \\ t - t_0 = \int dt &= \sqrt{\frac{m}{2E}} \int_{x_0}^{x} \frac{dx}{\sqrt{1 - \frac{U}{E}}} \end{aligned}$$

With $q = -\sqrt{\frac{2E}{m}}t_0$ this has the same form as the solution for q.

8.4.4 Example 4: Two dimensional oscillator as a central force

Suppose we have a mass fastened to a spring, moving on a tabletop, so that action is

$$S = \int \left(\frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\varphi}^2 \right) - \frac{1}{2} k r^2 \right)$$

The canonical momenta are

$$\begin{aligned} p_r &= m\dot{r} \\ p_\varphi &= m r^2 \dot{\varphi} \end{aligned}$$

so the Hamiltonian is

$$\begin{aligned} H &= \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\varphi}^2 \right) + \frac{1}{2} k r^2 \\ &= \frac{1}{2m} \left(p_r^2 + \frac{p_\varphi^2}{r^2} \right) + \frac{1}{2} k r^2 \end{aligned}$$

The Hamilton-Jacobi equation is

$$\frac{1}{2m} \left(\left(\frac{\partial \mathcal{S}}{\partial r} \right)^2 + \frac{1}{r^2} \left(\frac{\partial \mathcal{S}}{\partial \varphi} \right)^2 \right) + \frac{1}{2} k r^2 = -\frac{\partial \mathcal{S}}{\partial t}$$

Let $\mathcal{S} = f(r, \varphi) - Et$ to separate the time, so that

$$\frac{1}{2m} \left(\left(\frac{\partial \mathcal{S}}{\partial r} \right)^2 + \frac{1}{r^2} \left(\frac{\partial \mathcal{S}}{\partial \varphi} \right)^2 \right) + \frac{1}{2} k r^2 = E$$

Now use separation of variables. Let

$$f = R(r) + \Phi(\varphi)$$

Then

$$\begin{aligned} \left(\frac{dR}{dr} \right)^2 + \frac{1}{r^2} \left(\frac{d\Phi}{d\varphi} \right)^2 + kmr^2 &= 2mE \\ \left(\frac{dR}{dr} \right)^2 + kmr^2 - 2mE &= -\frac{1}{r^2} \left(\frac{d\Phi}{d\varphi} \right)^2 \\ -r^2 \left(\frac{dR}{dr} \right)^2 - kmr^4 + 2mEr^2 &= \left(\frac{d\Phi}{d\varphi} \right)^2 \end{aligned}$$

Since the left side depends only on r and the right only on φ, each side must equal some constant, a^2:

$$\begin{aligned} -r^2 \left(\frac{dR}{dr} \right)^2 - kmr^4 + 2mEr^2 - a^2 &= 0 \\ \frac{d\Phi}{d\varphi} &= \pm a \end{aligned}$$

We immediately integrated the equation for Φ:

$$\Phi = \pm a\varphi + b$$

To find R:

$$\begin{aligned}
-r^2\left(\frac{dR}{dr}\right)^2 - kmr^4 + 2mEr^2 - a^2 &= 0 \\
\frac{dR}{dr} &= \frac{1}{r}\sqrt{2mEr^2 - kmr^4 - a^2} \\
R &= \int \frac{dr}{r}\sqrt{2mEr^2 - kmr^4 - a^2} \\
&= \int \frac{rdr}{r^2}\sqrt{2mEr^2 - kmr^4 - a^2}
\end{aligned}$$

Let $z = r^2$,

$$R = \frac{1}{2}\int \frac{dz}{z}\sqrt{2mEz - kmz^2 - a^2}$$

Complete the square

$$2mEz - kmz^2 - a^2 = -\left(\frac{mE}{\sqrt{km}} - \sqrt{km}z\right)^2 + \frac{E^2}{\omega^2} - a^2$$

where $\omega = \sqrt{\frac{k}{m}}$. Then setting $y = \sqrt{km}z - \frac{mE}{\sqrt{km}}$, so that $\frac{y}{\sqrt{km}} + \frac{mE}{km} = z$

$$\begin{aligned}
R &= \frac{1}{2}\int \frac{dy}{\sqrt{km}\left(\frac{y}{\sqrt{km}} + \frac{E}{k}\right)}\sqrt{\left(\frac{E^2}{\omega^2} - a^2\right) - y^2} \\
&= \frac{1}{2}\int \frac{dy}{\left(y + \frac{E}{\omega}\right)}\sqrt{\left(\frac{E^2}{\omega^2} - a^2\right) - y^2}
\end{aligned}$$

Now let $y = \sqrt{\frac{E^2}{\omega^2} - a^2}\sin\theta$

$$\begin{aligned}
R &= \frac{1}{2}\int \frac{dy}{\sqrt{\left(\frac{E^2}{\omega^2} - a^2\right)}\sin\theta + \frac{E}{\omega}}\sqrt{\frac{E^2}{\omega^2} - a^2}\cos\theta \\
&= \frac{1}{2}\sqrt{\frac{E^2}{\omega^2} - a^2}\int \frac{dy}{\sin\theta + \frac{E}{\sqrt{(E^2 - a^2\omega^2)}}}\cos\theta \\
&= \theta - \frac{2a}{\sqrt{a^2-1}}\tan^{-1}\left(\frac{\frac{E}{\sqrt{(E^2-a^2\omega^2)}}}{\sqrt{\frac{E^2}{E^2-a^2\omega^2} - 1}}\left(\tan\left(\frac{\theta}{2}\right) + 1\right)\right) \\
&= \theta - \frac{2a}{\sqrt{a^2-1}}\tan^{-1}\left(\frac{E}{a\omega}\left(\tan\left(\frac{\theta}{2}\right) + 1\right)\right) \\
&= \theta - \frac{2a}{\sqrt{a^2-1}}\tan^{-1}\left(\frac{a\tan\left(\frac{\theta}{2}\right) + a}{\sqrt{a^2-1}}\right)
\end{aligned}$$

where

$$\theta = \sin^{-1}\left(\frac{m\omega^2 r^2 - E}{\sqrt{E^2 - a^2\omega^2}}\right)$$

Then

$$\mathcal{S} = R(r) + a\varphi - Et$$

9 Quantum Mechanics and the Hamilton-Jacobi equation

The Hamiltonian-Jacobi equation provides the most direct link between classical and quantum mechanics. There is considerable similarity between the Hamilton-Jacobi equation and the Schrödinger equation:

$$\begin{aligned}\frac{\partial \mathcal{S}}{\partial t} &= -H(x_i, \frac{\partial \mathcal{S}}{\partial x_i}, t) \\ i\hbar\frac{\partial \psi}{\partial t} &= H(\hat{x}_i, \hat{p}_i, t)\end{aligned}$$

We make the relationship precise as follows.

Suppose the Hamiltonian in each case is that of a single particle in a potential:

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$$

Write the quantum wave function as

$$\psi = Ae^{\frac{i}{\hbar}\varphi}$$

The Schrödinger equation becomes

$$\begin{aligned}i\hbar\frac{\partial\left(Ae^{\frac{i}{\hbar}\varphi}\right)}{\partial t} &= -\frac{\hbar^2}{2m}\bigtriangledown^2\left(Ae^{\frac{i}{\hbar}\varphi}\right) + V\left(Ae^{\frac{i}{\hbar}\varphi}\right) \\ i\hbar\frac{\partial A}{\partial t}e^{\frac{i}{\hbar}\varphi} - Ae^{\frac{i}{\hbar}\varphi}\frac{\partial\varphi}{\partial t} &= -\frac{\hbar^2}{2m}\bigtriangledown\cdot\left(e^{\frac{i}{\hbar}\varphi}\bigtriangledown A + \frac{i}{\hbar}Ae^{\frac{i}{\hbar}\varphi}\bigtriangledown\varphi\right) + VAe^{\frac{i}{\hbar}\varphi} \\ &= -\frac{\hbar^2}{2m}e^{\frac{i}{\hbar}\varphi}\left(\frac{i}{\hbar}\bigtriangledown\varphi\bigtriangledown A + \bigtriangledown^2 A\right) \\ &\quad -\frac{\hbar^2}{2m}e^{\frac{i}{\hbar}\varphi}\left(\frac{i}{\hbar}\bigtriangledown A\cdot\bigtriangledown\varphi + \frac{i}{\hbar}A\bigtriangledown^2\varphi\right) \\ &\quad -\frac{\hbar^2}{2m}\left(\frac{i}{\hbar}\right)^2 e^{\frac{i}{\hbar}\varphi}\left(A\bigtriangledown\varphi\cdot\bigtriangledown\varphi\right) \\ &\quad +VAe^{\frac{i}{\hbar}\varphi}\end{aligned}$$

Then cancelling the exponential,

$$\begin{aligned}i\hbar\frac{\partial A}{\partial t} - A\frac{\partial\varphi}{\partial t} &= -\frac{i\hbar}{2m}\bigtriangledown\varphi\cdot\bigtriangledown A - \frac{\hbar^2}{2m}\bigtriangledown^2 A \\ &\quad -\frac{i\hbar}{2m}\bigtriangledown A\cdot\bigtriangledown\varphi - \frac{i\hbar}{2m}A\bigtriangledown^2\varphi \\ &\quad +\frac{1}{2m}\left(A\bigtriangledown\varphi\cdot\bigtriangledown\varphi\right) + VA\end{aligned}$$

Collecting by powers of $\hbar$,

$$\begin{aligned}O\left(\hbar^0\right) &: \quad -\frac{\partial\varphi}{\partial t} = \frac{1}{2m}\bigtriangledown\varphi\cdot\bigtriangledown\varphi + V \\ O\left(\hbar^1\right) &: \quad \frac{1}{A}\frac{\partial A}{\partial t} = -\frac{1}{2m}\left(\frac{2}{A}\bigtriangledown A\cdot\bigtriangledown\varphi + \bigtriangledown^2\varphi\right) \\ O\left(\hbar^2\right) &: \quad 0 = -\frac{\hbar^2}{2m}\bigtriangledown^2 A\end{aligned}$$

The zeroth order terms is the Hamilton-Jacobi equation, with $\varphi = \mathcal{S}$:

$$\begin{aligned}-\frac{\partial\mathcal{S}}{\partial t} &= \frac{1}{2m}\bigtriangledown\mathcal{S}\cdot\bigtriangledown\mathcal{S} + V \\ &= \frac{1}{2m}\mathbf{p}^2 + V(x)\end{aligned}$$

where $p = \bigtriangledown \mathcal{S}$. Therefore, the Hamilton-Jacobi equation is the $\hbar \to 0$ limit of the Schrödinger equation.

$$H\psi = \frac{p^2}{2m}\psi + V\left(x\right)\psi$$