Hamiltonian Mechanics

The principle of least action states that the path followed by a system is that which extremizes the action

$$J(q) = \int_{t_1}^{t_2} L(q, \dot{q}, t) \, dt$$

where the Lagrangian $L = T - U$. This results in the equations of motion:

$$\left(1 \right) \quad \frac{\partial L}{\partial \dot{q}_i} - \frac{d}{dt} \frac{\partial L}{\partial q_i} = 0$$

These are $n$ coupled 2nd order differential equations for $q_i(t)$.

Recall the momenta $p_i$ conjugate to $q_i$ are defined by

$$\left(2 \right) \quad p_i = \frac{\partial L}{\partial \dot{q}_i} (q, \dot{q}, t) \quad i = 1, \ldots n$$

This should be regarded as a set of $n$ coupled (algebraic) equations defining a transformation

$$p \leftrightarrow q$$

In Hamiltonian mechanics one views the solution (motion) as one in $(q, p)$ phase space and reformulates (1).
Given the definition of $p_i$ the EL-eqns (1):

\[ \frac{dp_i}{dt} = \frac{\partial L}{\partial q_i'}(q, q', t) \]

In so much as (2) yields an invertible transformation $p \leftrightarrow q$ then the right side of (3) is a function of $(q, p')$.

**Hamiltonian Definition**

\[ H \equiv \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L = \dot{q}_i p_i - L \]

**Conservation of $H$:** (Assume $L_t = 0$)

\[ \frac{d}{dt}(\dot{q}_i p_i - L) = \ddot{q}_i \frac{\partial L}{\partial \dot{q}_i'} + \dot{q}_i \frac{\partial L}{\partial \dot{q}_i'} \frac{\partial \dot{q}_i}{\partial q_i} - \frac{\partial L}{\partial q_i'} \frac{\partial \dot{q}_i}{\partial q_i} 
\]

Hence

\[ \frac{dH}{dt} = 0 \]

is a constant of the motion.

If $L_t \neq 0$ then similar calculations yield

\[ \frac{dH}{dt} = -\frac{\partial L}{\partial t} \]
Hamiltonian and Energy.

If $x$ are the cartesian coordinates for a system and $q$ the generalized coordinates, there exists $T_{ij}(q)$ such that the kinetic energy

$$T(q, \dot{q}) = \sum_{ij} T_{ij}(q) \dot{q}_i \dot{q}_j$$

**Ex.** For the spherical pendulum

$$T = \frac{1}{2} m R^2 \left( \sin^2 \phi \dot{\phi}^2 + \dot{\theta}^2 \right)$$

wlog $mR^2=2$ so that for $q = (\theta, \phi)$

$$\begin{bmatrix} T_{ij} \end{bmatrix} = \begin{bmatrix} \sin^2 \phi & 0 \\ 0 & 1 \end{bmatrix}$$

**Defn.** A function $F(q, \dot{q})$ is homogeneous of degree $n$ if

$$F(q, \alpha \dot{q}) = \alpha^n F(q, \dot{q}) \quad \forall \alpha \in \mathbb{R}$$

**Lemma.** Since $T(q, \dot{q})$ is homogeneous of degree $n = 2$

$$\dot{q}_i \frac{\partial T}{\partial \dot{q}_i} = n T$$

**Pf.** Define $F(q) = T(q, \alpha \dot{q})$ and compute $F'(q)$

$$F'(1) = \frac{\partial T}{\partial \dot{q}_i} \dot{q}_i = n T(q, \dot{q})$$

[chain rule defn of homog]
Theorem: If $\frac{\partial U}{\partial q_i} = 0$ then $H = T + U$

Proof:

$$H = \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L$$

by lemma

$$H = 2T - L$$

$$H = T + U$$

Summary:

(1) $\frac{dH}{dt} = -\frac{\partial L}{\partial t}$

(2) $H = T + U$ if $U = U(q)$

Remark: if $L_t = 0$ then $H$ conserved.
Hamiltons Equations

Seek eqns for \((q, p) \in \mathbb{R}^{2n}\) that extremize the action

\[
\mathcal{J}(q) = \int_{t_1}^{t_2} \left( \sum_l p_l \dot{q}_l - H(q, p) \right) \, dt
\]

where the system

\[
\dot{p}_i = \frac{\partial L}{\partial \dot{q}_i}(q, \dot{q})
\]

(2) defines a transformation \((q, \dot{q}) \leftrightarrow (q, p)\).
As such \(q_i\) may be viewed as function of \((q, p)\). Now note

\[
dL = \frac{\partial L}{\partial q_i} \, dq_i + \frac{\partial L}{\partial \dot{q}_i} \, d\dot{q}_i + \frac{\partial L}{\partial t} \, dt
\]

Using the EL-eqns and (2)

\[
dL = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) dq_i + p_i \, dq_i + \frac{\partial L}{\partial t} \, dt
\]

or

\[
dL = p_i \, dq_i + \dot{p}_i \, d\dot{q}_i + \frac{\partial L}{\partial t} \, dt
\]

(3) \[
dL = \dot{p}_i \, dq_i + d(q_i \dot{q}_i) - \dot{q}_i \, dp_i + \frac{\partial L}{\partial t} \, dt
\]

Indicated terms in (3) can be written as a differential of the Hamiltonian.
Rearranging

\[ d\left(\frac{p_i q_i - L}{H}\right) = -\dot{p}_i \, dq_i + \dot{q}_i \, dp_i - \frac{\partial L}{\partial t} \, dt \]

Hence

\[ dH = \frac{\partial H}{\partial q_i} \, dq_i + \frac{\partial H}{\partial p_i} \, dp_i = -\dot{p}_i \, dq_i + \dot{q}_i \, dp_i - \frac{\partial L}{\partial t} \, dt \]

Matching differentials we arrive at Hamilton's equations for the motion

\[
\begin{align*}
\dot{q}_i &= \frac{\partial H}{\partial p_i} \\
\dot{p}_i &= -\frac{\partial H}{\partial q_i} \\
\frac{dH}{dt} &= -\frac{\partial L}{\partial t}
\end{align*}
\]

Again note \( H \) is conserved if \( L_t = 0 \).
Alternate derivations

We shall accept the first of Hamilton's equations (hard to prove)

\[ q_i = \frac{\partial H}{\partial p_i} \]

and derive the second equation for \( \dot{p}_i \)

For clarity we define \((q, \dot{q}) \leftrightarrow (Q, P)\) by

\[ Q_i = q_i \quad P_i = \frac{\partial L}{\partial \dot{q}_i} (Q, \dot{q}) \]

so that \( H = H(Q, P) \). Then

\[
\frac{\partial H}{\partial q_i} = \frac{\partial H}{\partial p_k} \frac{\partial p_k}{\partial q_i} + \frac{\partial H}{\partial Q_i}
\]

\[
= -q_i \frac{\partial p_k}{\partial q_i} + \frac{\partial H}{\partial Q_i}
\]

\[
= \frac{\partial}{\partial q_i} \left( H - q_k p_k \right)
\]

\[
= -\frac{\partial L}{\partial q_i}
\]

\[
= -\frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}_i} \right)
\]

\[
= -\dot{p}_i
\]

Hence

\[ \dot{p}_i = -\frac{\partial H}{\partial q_i} \]
Example: Cartesian coordinates \( x = (x_1, x_2, x_3) \)

Derive Hamiton's equations for a particle of mass \( m \) with potential \( V = V(x) \).

\[
T = \frac{1}{2} m (\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2) = \frac{1}{2} m \| \dot{x} \|^2
\]

Determine conjugate momenta from lagrangian

\[
L = T - U = \frac{1}{2} m (\dot{x}_i)^2 - U(x)
\]

Since \( \dot{V}_x = 0 \) the Hamiltonian is \( H = T + V \n
\[
p_i \equiv \frac{\partial L}{\partial \dot{x}_i} = m \dot{x}_i
\]

So that

\[
\dot{x}_i = \frac{1}{m} p_i
\]

and

\[
H = \frac{1}{2m} (p_1^2 + p_2^2 + p_3^2) + V(x)
\]

Hamilton's eqns are

1. \[
\dot{x}_i = \frac{\partial H}{\partial p_i} = \frac{1}{m} p_i
\]

2. \[
\dot{p}_i = -\frac{\partial H}{\partial x_i} = -\frac{\partial V}{\partial x_i}
\]

The second equation implies \( \dot{p} = -\nabla U \). The first yields the standard defn of momentum \( p_i = m \dot{x}_i \). Collectively

\[
\frac{d}{dt} (m \dot{x}_i) = -\frac{\partial V}{\partial x_i}
\]

\[
\frac{dp}{dt} = -\nabla V
\]
EXAMPLE
A bead of mass m slides frictionlessly on a cone
\[ a z = \sqrt{x^2 + y^2} \text{ where } a \in \mathbb{R} \]

Choose cylindrical coordinates as the generalized coordinates.

\[ q = (r, \theta, z) \]

The problem has a holonomic constraint

\[ (1) \quad \Gamma = a z \]

We seek to find Hamilton's eqns for motion. Need to express \( T = T(q, \dot{q}) \) and then find \( p \) from EL-eqns. Use (1) and

\[
\begin{align*}
x &= r \cos \theta = a z \cos \theta \\
y &= r \sin \theta = a z \sin \theta
\end{align*}
\]

Then after some calculations

\[ T = \frac{1}{2} m (x^2 + y^2 + z^2) = \frac{1}{2} m \left( (1 + a^2) \dot{z}^2 + a^2 z^2 \dot{\theta}^2 \right) \]

Lagrangian is

\[ (1) \quad L = \frac{1}{2} \left[ (1 + a^2) \dot{z}^2 + a^2 z^2 \dot{\theta}^2 \right] - mg z \]

where gravitational \( U = mg z \).
Conjugate momenta \( p = (p_z, p_\theta) \)

\[ p_z = \frac{\partial L}{\partial \dot{z}} = m(1 + a^2) \dot{z} \]

\[ p_\theta = \frac{\partial L}{\partial \dot{\theta}} = ma^2 z^2 \dot{\theta} \]

Here \( q = (z, \theta) \) and \( \dot{q} = (\dot{z}, \dot{\theta}) \). Eqns (2)-(3) define a transformation \((q, \dot{q}) \leftrightarrow (p, \dot{p})\).

Since \( \mathcal{L}_q = 0 \), \( H = T + V \). Since \( T \) is computed already, we use (2)-(3) to eliminate \((\dot{z}, \dot{\theta})\) to get

\[ H = T + V = \frac{p_z^2}{2m(1 + a^2)} + \frac{p_\theta^2}{2ma^2 z^2} + mgz \]

Hence we get the four Hamilton's eqns

\[ p_\theta = -\frac{\partial H}{\partial \theta} = 0 \]

\[ \dot{p}_z = -\frac{\partial H}{\partial z} = -mg + \frac{p_\theta^2}{ma^2 z^3} \]

\[ \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ma^2 z^2} \]

\[ \dot{z} = \frac{\partial H}{\partial p_z} = \frac{p_z}{m(1 + a^2)} \]

Conserved Quantities

\[ \dot{p}_\theta = 0 \quad \text{eqn (5) above} \]

\[ \dot{H} = 0 \quad \frac{\partial L}{\partial t} = 0 \]

Values of these constants found from \( q(0), \dot{q}(0) \) in (2)-(3) and defn of \( H \).
Solving the eqns of motion.

Differentiate eqn (8) in $t$ and use (6):

$$ (9) \quad \ddot{z} + F(z) = 0 $$

where $F(z) = \alpha - \beta z^{-3}$ for $\alpha, \beta > 0$ given by

$$ \alpha = \frac{g}{1+a^2}, \quad \beta = \frac{p_0^2}{m^2a^2(1+a^2)} $$

Note $\beta$ is constant.

Eqns like (9) frequently arise in mechanics.

$$ \ddot{z} \dot{z} + F(z) \dot{z} = 0 $$

$$ \frac{d}{dt} \left( \frac{1}{2} \dot{z}^2 + f(z) \right) = 0 \quad f(z) = \dot{z} \dot{z} + \frac{1}{2} \beta \dot{z}^{-2} $$

$$ (10) \quad \frac{1}{2} \dot{z}^2 + f(z) = E $$

for some constant $E$. This eqn is not a surprise since $H$ is constant. Can re-derive (10) using (8) in (4) to eliminate $p_z$.

Basically, there are four eqns of motion and two constants of the motion so one expects a reduction to a single 2nd equation like (10). Solving (10) amounts to the following quadrature

$$ \int \frac{z \, dz}{\sqrt{2Ez^2 - 2\alpha z^3 + \beta}} = dt \quad \text{(sadly not doable)} $$
**Example: Central Forces**

In spherical coordinates \( q = (r, \theta, \phi) \) where \( \theta \in [0, 2\pi] \) and \( \phi \in [0, \pi] \).

\[
L = T - U = \frac{1}{2} m r^2 + \frac{1}{2} m r^2 \dot{\theta}^2 + \frac{1}{2} m r^2 \sin^2 \theta \dot{\phi}^2 - U(r)
\]

**Conjugate momenta**

1. \( p_r = \frac{\partial L}{\partial \dot{r}} = m \dot{r} \)
2. \( p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m r^2 \dot{\theta} \)
3. \( p_\phi = \frac{\partial L}{\partial \dot{\phi}} = m r^2 \sin^2 \theta \dot{\phi} \) (conserved)

Note that (1)-(3) define \((q, \dot{q}) \leftrightarrow (q, p)\)

Since \( L \dot{\phi} = 0 \) the EL-eqns \( \Rightarrow p_\phi \) is constant. And, since \( L_t = 0 \), the previous theorem implies the Hamiltonian is also constant. Moreover \( \frac{\partial H}{\partial \dot{t}} = 0 \) implies \( H = T + U \)

Using (1)-(3) to eliminate \( \dot{\phi} \) we find

\[
H = \frac{1}{2m} \left\{ \frac{p_r^2}{r^2} + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2 \sin^2 \theta} \right\} + U(r)
\]
Just to be explicit we list all six of Hamilton's eqns.

\( \dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m} \)

\( \dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{m r^2} \)

\( \dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi}{m r^2 \sin^2 \theta} \)

and associated momenta eqns

\( \dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_\theta^2}{m r^3} + \frac{p_\phi^2}{m r^3 \sin^2 \theta} - \frac{\partial U}{\partial r} \)

\( \dot{p}_\theta = -\frac{\partial H}{\partial \theta} = \frac{p_\phi^2 \cos \theta}{m r^2 \sin^3 \theta} \)

\( \dot{p}_\phi = -\frac{\partial H}{\partial \phi} = 0 \)

Phase space \((q, p) \in \mathbb{R}^6\).

Note that for orbital motion on \( \phi = \phi_0 \)
we have \( \dot{\phi} = 0 \), \( p_\phi = 0 \) and indicated terms vanish. Then \( p_\theta \) is constant
and \((1), (4)\) yield \((2)\) for constant \( m \)

\[ m \ddot{r} = \frac{p_\theta^2}{m r^3} - \frac{\partial U}{\partial r} = F(r) \]

which in principle is integrable.
EXAMPLE  Velocity dependent potential

The Lorenz force acting on a particle of charge $e$ under the influence of electric field $\vec{E}$ and magnetic field $\vec{B}$ is

$$\vec{F} = e \left( \vec{E} + \vec{v} \times \vec{B} \right)$$

where $\vec{v}$ is velocity (cartesian).

From the theory of electromagnetism

$$\vec{E} = -\nabla \phi - \frac{\partial \vec{A}}{\partial t} \quad \vec{B} = \nabla \times \vec{A}$$

where

$\phi = \text{scalar electric potential}$

$\vec{A} = \text{vector magnetic potential}$

The associated "potential energy" is for cartesian coordinates $q$

$$\mathcal{U}(q, \dot{q}, t) = e \left( \phi - \dot{q}_i A_i \right) \quad *$$

with the resulting Lagrangian

$$L = \frac{1}{2} m \dot{q}_i^2 - e \left( \phi - \dot{q}_i A_i \right)$$

$$L = \frac{1}{2} m \| \dot{q} \|^2 - e \phi + e \dot{q} \cdot A$$

* show this yields (1) via Eqs. for $A_z = 0, A_q = 0$
As long as $L_x = 0$ the Hamiltonian is still conserved. However $V$ depends on $q$ so the theorem which assures $H = T + V$ is no longer valid and one must use

\[(3) \quad H(q, p) = \dot{q}_i p_i - L(q, \dot{q}, t)\]

where conjugate momenta are

\[(4) \quad p_i = \frac{\partial L}{\partial \dot{q}_i} = m \dot{q}_i + eA_i\]

or in vector form

\[p = m \dot{q} + eA\]

We use (4) to eliminate $\dot{q}_i$ in (3). After some calculations one obtains (* show) a simple vector form the Hamiltonian.

\[H = \frac{1}{2m} (p - eA) \cdot (p - eA) + e \varphi\]

This is the correct form for quantum mechanics. Hamilton's equations are a tad messy.
**Canonical Transformations**

Is any transformation \((p, q, t) \leftrightarrow (P, Q, t)\) for which Hamilton's equations remain invariant?

\[
h(p, q, t) = \text{old Hamiltonian} \\
H(P, Q, t) = \text{new Hamiltonian}
\]

Define old and new actions

\[
s(p, q) = \int (p_i q_i - h) \, dt \\
S'(P, Q) = \int (P_i Q_i - H) \, dt
\]

Note \(Ss = 0\) and \(Ss = 0\) simultaneously if the actions differ by an exact differential, or that \(\exists F\) s.t.

\[
(1) \quad p_i q_i - h = P_i Q_i - H + \frac{dF}{dt}
\]

Many choices but one is

\[
(2) \quad F = F_2(q, P, t) - P_i Q_i
\]

For such \(F\), eqn (1) is true if

\[
(3) \quad P_i = \frac{\partial F_2}{\partial q_i} (q, P, t) \\
(4) \quad Q_i = \frac{\partial F_2}{\partial P_i} (q, P, t) \\
(5) \quad H = h + \frac{\partial F_2}{\partial t}
\]

implicitly define \((q, p) \leftrightarrow (Q, P)\)
Hamilton Jacobi Theory

Seek a canonical transformation so the new Hamiltonian \( H = 0 \). In that case

\[
\dot{Q}_i = 0 \quad \dot{P}_i = 0
\]

so \( Q_i, P_i \) are 2n constants of the motion. In doing so, one would have solved the equations of motion.

Using (5) and (6) the transformation which accomplishes this goal satisfies the Hamilton-Jacobi eqn (PDE)

\[
H = h(q_1, q_2, \ldots, \frac{\partial F_1}{\partial q_1}, \ldots, \frac{\partial F_2}{\partial q_n}, t) + \frac{\partial F_2}{\partial t} = 0
\]

where \( p_i = \dot{q}_i \) constant. Any soln will do.

**Example** \( h(q, p) = \frac{1}{2m} (p^2 + m^2 \omega^2 q^2) \) Harm. Osc.

Hamilton Jacobi equation \( F_2 = S \) is

\[
\frac{1}{2m} \left( \left( \frac{\partial S}{\partial q} \right)^2 + m^2 \omega^2 q^2 \right) + \frac{\partial S}{\partial t} = 0
\]

Letting \( S(q, \dot{q}, t) = W(q, \dot{q}) - \dot{q} \dot{t} \) yields

\[
\left( \frac{\partial W}{\partial q} \right)^2 + m^2 \omega^2 q^2 = 2md,
\]

which is a separable, solvable first order nonlinear ODE for \( W \).
Generating functions and waves

Suppose \( H \) is conserved and \( H = E \) is the energy. Let \( S(q, p, t) \) be the generating function that solves the Hamilton-Jacobi Eqn. \((\mathcal{HJ})\)

\[
S(q, p, t) = W(q, p) - Et
\]

Then \( W(q, p) = \text{constant} \) are surfaces in \((p, q)\) phase space.

\[
\begin{align*}
W &= a \\
W &= a + E dt = a + dW
\end{align*}
\]

Wave front velocity

\[
u = \frac{ds}{dt}
\]

Hamilton-Jacobi equation for one-particle

\[
\frac{1}{2m} \| \nabla W \|^2 + V = E
\]

where \( E = \text{energy} \) and \( V = \text{potential energy} \).

Since \( p_i = \frac{\partial W}{\partial q_i} \).
Schrödinger Eqn.

\[ \frac{\hbar^2}{2m} \nabla^2 \psi - V \psi = \frac{i}{\hbar} \frac{\partial \psi}{\partial t} \]

If one lets

\[ \psi(q, t) = \psi_0 \exp \left( \frac{i \mathcal{S}/\hbar} \right) \]

you get

\[ \frac{1}{2m} (\nabla \mathcal{S})^2 + V + \frac{\partial \mathcal{S}}{\partial t} = \frac{i k \nabla^2 \mathcal{S}}{2m} \]

Very close. Equal to H\S if (RHS) = 0 !!

when does this happen?

\[ \hbar \nabla^2 \mathcal{S} \ll |\nabla \mathcal{S}|^2 \]

But \( p_i = \frac{\partial \mathcal{S}}{\partial q_i} \) so same as

\[ \hbar \nabla \cdot p \ll p^2 \]

\[ \frac{\hbar dp}{p dx} \ll 1 \quad \text{one dim.} \]