Legendre Transform

Let consider the simple case with just a real value function: \( F(x) \)

\( F(x) \) expresses a relationship between an independent variable \( x \) and its dependent value \( F \)

\( \Rightarrow \) This relation is encoded in the functional form of \( F(x) \)

\( \Rightarrow \) We will denote this encoding in general by: \( \{F, x\} \)

As one has learned in math and physics, it is sometime useful to encode the information contained in a function in different ways...

\( \vdots \)

\( \Rightarrow \) e.g., Fourier Transform, Laplace Transform, etc.
Legendre Transform

As in the Fourier Transform:  
\[ \hat{F}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} F(x) \, dx \]

and its inverse transform:  
\[ F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{+ikx} \hat{F}(k) \, dk \]

→ The original information of \( F(x) \) for a given \( x \) value is encoded in terms of the Fourier components \( \hat{F}(k) \) and a new set of variables \( k \).

→ In our new encoding scheme, we will say that  
\[ \{\hat{F}, k\} \text{ encodes the SAME information as } \{F, x\} \]
Legendre Transform

The Legendre Transform is yet another (convenient) encoding scheme for \( F(x) \) when the following two conditions are true:

1. The function is strictly convex (concave), i.e., 2\(^{nd}\) derivative always positive (negative) and smooth

2. It is easier to measure, control, or think about \( \frac{dF}{dx} \) than \( x \) itself

\( \rightarrow \) Since \( \frac{dF}{dx} \) never changes sign (condition 1), there is a one-to-one correspondence between \( \frac{dF}{dx} \) and \( x \)

\( \rightarrow \) Legendre Transform gives us a new encoding scheme \( \{G, s\} \) with \( G(s) \) being a function of \( s = \frac{dF}{dx} \) instead of \( x \)
Legendre Transform

Here is the definition of the Legendre Transform for \( F(x) \)

\[
G(s) = sx(s) - F(x(s))
\]

Note that \( G(s) \) is a function of \( s \) and we have to express \( F(x(s)) \) in terms of \( s \) by inverting the function: \( s = \frac{dF(x)}{dx} \) to get \( x(s) \)
Legendre Transform

Geometric Construction of the Legendre Transform: \( G = sx - F \)

![Image showing the geometric construction of the Legendre Transform. The graph illustrates the relationship between the functions \( F(x) \) and \( G \), with \( F(x) \) being translated by the slope \( s \) to obtain \( G \). The y-intercept of the slope \( s \) is shown, and the equation \( F + G = sx \) is indicated.]
Legendre Transform

Important Properties of the Legendre Transform:

1. The Legendre Transform is its own inverse transform:

   - Suppose we have \( G(s) \) and define \( y(s) = \frac{dG(s)}{ds} \)

   - Using the inverted relation \( s(y) \), the Legendre Transform of \( G(s) \) is

     \[ H(y) = y_s(y) - G(s(y)) \]

   - This can be rewritten as \( G = sy - H \) and comparing to our original transform \( G = sx - F \), we can immediate see that \( \{H, y\} = \{F, x\} \)

     and \( F = xs - G \) is \( F \)'s own inverse transform.
Legendre Transform

- The two independent variables \((x, s)\) are two *conjugate* pair of variables related to each other through

\[
x(s) = \frac{dG(s)}{ds} \quad \text{or} \quad s(x) = \frac{dF(x)}{dx}
\]

- Note that there is only ONE independent variable (either \(x\) or \(s\)) in:

\[
F(x) + G(s(x)) = s(x)x
\]

\[
F(x(s)) + G(s) = sx(s)
\]
Legendre Transform

2. Properties of the Minima [note: \( F(x) \) is convex, an extrema is a minimum]

At the minimum \( F_{\text{min}} \) of \( F(x) \) we have the slope

\[
s = \frac{dF}{dx} = 0
\]

So, we have

\[
G(s = 0) = x \cdot 0 - F_{\text{min}}
\]

\[
F_{\text{min}} = -G(0)
\]
Legendre Transform

2. Properties of the Minima

Similarly, at a minimum \( G_{\min} \) of \( G(s) \)
We again have correspondingly

\[
\frac{dG}{ds} (\text{slope for } G) \equiv x = 0
\]

So, we have

\[
G_{\min} = -F(0)
\]
Legendre Transform

2. Reciprocal Relation of $F$ & $G$’s curvature

Start with the two reciprocal definitions

$$x(s) = \frac{dG(s)}{ds} \quad \text{and} \quad s(x) = \frac{dF(x)}{dx}$$

Now take derivatives with respect to their independent variables,

$$\frac{dx}{ds} = \frac{d^2G(s)}{ds^2} \quad \otimes \quad \frac{ds}{dx} = \frac{d^2F(x)}{dx^2}$$

$$\left(\frac{d^2F(x)}{dx^2}\right)\left(\frac{d^2G(s)}{ds^2}\right) = \frac{ds}{dx} \frac{dx}{ds} = 1$$

So, if $F(x)$ is with curvature $\alpha$, then $G(s)$ will have curvature $1/\alpha$
Review of Lagrangian Formulation

Recall Lagrangian Formulation of Mechanics

- Pick \( n \) proper (independent) generalized coordinates to describe the state of the system \( \rightarrow \) this defines a \( n \)-dim Configuration Space.

- Apply the Hamilton’s Principle:

The motion of the system from \( t_1 \) to \( t_2 \) in config. space is such that the Action \( (I) \) has a stationary value, i.e.,

\[
\delta I = \delta \int_{1}^{2} L(q_j, \dot{q}_j, t) \, dt = 0
\]

- Using Variational Calculus, this implies the Euler-Lagrange Eq:

\[
\frac{\partial L}{\partial q_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) = 0, \quad j = 1, \ldots, n
\]
Review of Lagrangian Formulation

\[ \frac{\partial L}{\partial q_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) = 0, \quad j = 1, \ldots, n \]

→ Solving this gives the Equations of Motion

Notes:

- We have \( n \) independent generalized coordinates \( \{q_j\}_1^n \).
- The \( n \) \( \{\dot{q}_j\}_1^n \) are time derivatives of the \( \{q_j\}_1^n \).
- We have \( n \) 2\textsuperscript{nd}-order ODEs for the equations of motion
- We need \( 2n \) initial conditions to completely specify the motion.
Hamiltonian Formulation

- Instead of $n$ 2\textsuperscript{nd}-order ODEs as EOM with $n$ independent generalized coordinates in configuration space.
- Seek $2n$ 1\textsuperscript{st}-order ODEs as EOM with $2n$ independent generalized coordinates in phase space.

(Note: In Hamiltonian Formulation, we need to start with a set of independent generalized coordinates. If they are not proper, a reduced set of $m < n$ proper coordinates must be chosen first.)

- The most natural choice for this set of $2n$ variables in phase space is:

\[
\left\{ q_j \right\}_1^n \oplus \left\{ p_j \right\}_1^n \quad \text{where} \quad p_j \equiv \frac{\partial L}{\partial \dot{q}_j}
\]

generalized coordinates \hspace{1cm} \text{generalized conjugate momenta}
Hamiltonian Formulation

Notes:

- As we will see... this is NOT the only choice

- Coordinates in this $2n$-dim phase space are call “canonical variables”

(In Landau & Lifshitz: they are called “canonical” since the EOM resulted from them has the simplicity and symmetry in form.)

- Later, we will investigate invariant ways to transform the system to other $2n$ canonical variables using “canonical transformations”
Configuration Space vs. Phase Space

1. A given point in configuration space \( (q_1, \cdots, q_n) \) prescribes fully the “configuration” of the system at a given time \( t \).

- However, the specification of a point in this space does NOT specify the time evolution of the system completely!

  (a unique soln for a \( n \)-dim 2\(^{nd} \) order ODE needs \( 2n \) ICs)

- Many different paths can go thru a given point in config space

\[ \begin{align*}
\dot{q}_j &
\end{align*} \]

\[ \begin{align*}
\text{Different paths crossing } P \text{ will have the same set of } \{q_j\}_1^n \text{ but diff } \{\dot{q}_j\}_1^n
\end{align*} \]
Configuration Space vs. Phase Space

To specify the state AND time evolution of a system uniquely at a given time, one needs to specify BOTH \( \{q_j\} \) AND \( \{\dot{q}_j\} \) or equivalently, \( \{q_j, p_j\} \).

\[ \Rightarrow \text{The 2n-dim space where both } \{q_j\} \text{ and } \{p_j\} \text{ are independent variables is called phase space.} \]

\[ \Rightarrow \text{Thru any given point in phase space, there can only be ONE unique path!} \]
Hamiltonian Formulation

- Instead of using the Lagrangian, \( L = L(q_j, \dot{q}_j, t) \), we will introduce a new function that depends on \( q_j, p_j \), and \( t \): \( H = H(q_j, p_j, t) \)

- This new function is call the Hamiltonian and it is defined by:

\[
H = \frac{\partial L}{\partial \dot{q}_j} \dot{q}_j - L
\]

(Einstein’s Convention: Repeated indices are summed)

- Plugging in the definition for the generalized momenta: \( p_j \equiv \frac{\partial L}{\partial \dot{q}_j} \)

\[
H = p_j \dot{q}_j - L
\]

(sum)

→ One can think of this as a coordinate transformation from \((q_j, \dot{q}_j)\) to \((q_j, p_j)\)

To be more specific, \( H(q, p) \) is the Legendre Transform of \( L(q, \dot{q}) \).
→ \( H \) is defined “similarly” to the Jacobi (energy) function \( h \) BUT \( h \) is a function of \((q_j, \dot{q}_j)\) and \( H \) is a function of \((q_j, p_j)\).
\( L \) and \( H \) are a Legendre Transform Pair

Consider a simple Lagrangian for a single particle \( m \) under the influence of a conservative potential \( V(q) \)

\[
L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q)
\]

Then, we have \( p \equiv \frac{\partial L}{\partial \dot{q}} = m\dot{q} \)

Inverting the above relation and arriving at \( \dot{q}(p) = p/m \)

Then, the Legendre Transform of \( L(q, \dot{q}) \) is: \( \{L, \dot{q}\} \Leftrightarrow \{H, p\} \)

\[
H(q, p) = p\dot{q}(p) - L(q, \dot{q}(p)) \quad \text{(} \dot{q} \text{ is an irrelevant variable in this L-Trans)}
\]

\[
= p\left(\frac{p}{m}\right) - \frac{m}{2}\left(\frac{p}{m}\right)^2 + V(q) = \frac{p^2}{2m} + V(q)
\]
Hamiltonian Formulation

- Taking the differential of our definition for  \( H = p_j \dot{q}_j - L \), we have
  \[
dH = p_j d\dot{q}_j + \dot{q}_j dp_j - dL
  \]
  \( \text{(sum)} \)

- Now, we require that  \( H = H(q_j, p_j, t) \) so that we should have
  \[
dH = \frac{\partial H}{\partial q_j} dq_j + \frac{\partial H}{\partial p_j} dp_j + \frac{\partial H}{\partial t} dt
  \]
  \( \text{(sum)} \)

- To be consistent, let try to resolve this by expanding  \( dL \):
  \[
dL = \frac{\partial L}{\partial q_j} dq_j + \frac{\partial L}{\partial \dot{q}_j} d\dot{q}_j + \frac{\partial L}{\partial t} dt
  \]
  \( \text{(sum)} \)

- Plug in  \( p_j = \frac{\partial L}{\partial \dot{q}_j} \):
  \[
dL = \frac{\partial L}{\partial q_j} dq_j + p_j d\dot{q}_j + \frac{\partial L}{\partial t} dt
  \]
  \( \text{(sum)} \)
Hamiltonian Formulation

- Now, since the system satisfies the Euler-Lagrange Equation, we have

\[
\frac{\partial L}{\partial q_j} = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) = \dot{p}_j
\]

(\text{** this is an important step if we want our formalism to describe the same dynamic.**})

- Substituting this into our previous equation, we have:

\[
dL = \dot{p}_j dq_j + p_j d\dot{q}_j + \frac{\partial L}{\partial t} dt
\]

\text{(sum)}

- Now, plug this into our equation for \(dH:\)

\[
dH = \dot{p}_j d\dot{q}_j + \dot{q}_j dp_j - \dot{p}_j dq_j - p_j d\dot{q}_j - \frac{\partial L}{\partial t} dt
\]

\[
dH = \dot{q}_j dp_j - \dot{p}_j dq_j - \frac{\partial L}{\partial t} dt
\]

\text{(sum)}
Hamiltonian Formulation

- If $H$ describes the same dynamics as is given by the EL equation, the two expressions must equal to each other:

$$dH = -\dot{p}_j dq_j + \dot{q}_j dp_j - \frac{\partial L}{\partial t} dt$$

$$dH = \frac{\partial H}{\partial q_j} dq_j + \frac{\partial H}{\partial p_j} dp_j + \frac{\partial H}{\partial t} dt$$

- Comparing gives the condition:

$$\begin{align*}
\frac{\partial H}{\partial q_j} &= -\dot{p}_j \\
\frac{\partial H}{\partial p_j} &= \dot{q}_j
\end{align*}$$

\text{and}

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

These are called the Hamilton’s Equations of Motion and they are the desired set of equations describing the EOM in phase space.
Hamiltonian Formulation

Summary of Steps:

1. Pick a proper set of $q_j$ and form the Lagrangian $L$
2. Obtain the conjugate momenta by calculating $p_j \equiv \frac{\partial L}{\partial \dot{q}_j}$
3. Form $H = p_j \dot{q}_j - L$
4. Eliminate $\dot{q}_j$ from $H$ using the inverse of $p_j \equiv \frac{\partial L}{\partial \dot{q}_j}$ so as to have $H = H(q_j, p_j, t)$
5. Apply the Hamilton’s Equation of Motion:

$$\frac{\partial H}{\partial q_j} = -\dot{p}_j \quad \text{and} \quad \frac{\partial H}{\partial p_j} = \dot{q}_j$$

As you will see, this formulation does not necessary simplify practical calculations but it forms a theoretical bridge to QM and SM.
Hamilton Equations in Matrix (Symplectic) Notation

The pair of Hamilton equations look almost symmetric (except the “-” sign).

The following is an elegant way to write the Hamilton equations into a single matrix equation:

For a system with $n$ dofs, we group all of our $q_i$’s and $p_i$’s into a $2n$-dim vector $\eta$:

$$\eta_j = q_j, \quad \eta_{j+n} = p_j; \quad j = 1, \cdots, n$$

Similarly, we will define another $2n$-dimensional column vector $\partial H / \partial \eta$:

$$\begin{bmatrix} \frac{\partial H}{\partial \eta_j} \\ \frac{\partial H}{\partial \eta_{j+n}} \end{bmatrix} = \begin{bmatrix} \frac{\partial H}{\partial q_j} \\ \frac{\partial H}{\partial p_j} \end{bmatrix}; \quad j = 1, \cdots, n$$
Hamilton Equations in Matrix (Symplectic) Notation

Now, we define a $2n \times 2n$ anti-symmetric matrix $J$,

$$
J = \begin{pmatrix}
0 & I \\
-I & 0
\end{pmatrix}
$$

where $I$ is a $n \times n$ identity matrix

$0$ is a $n \times n$ zero matrix

Note that the transpose of $J$ is its own inverse (orthogonal):

$$
J^T = \begin{pmatrix}
0 & -I \\
I & 0
\end{pmatrix}
$$

and

$$
J^T J = JJ^T = \begin{pmatrix}
I & 0 \\
0 & I
\end{pmatrix}
$$

In summary, we have the following properties for $J$:

$$
J^T = -J = J^{-1}, \quad J^2 = -I, \quad \det(J) = +1
$$
Hamilton Equations in Matrix (Symplectic) Notation

The Hamilton equation can then be written in a compact form:

\[
\dot{\eta} = J \frac{\partial H}{\partial \eta}
\]

As an example, with only 2 dofs, this matrix equation expands into:

\[
\begin{pmatrix}
\dot{q}_1 \\
\dot{q}_2 \\
\dot{p}_1 \\
\dot{p}_2
\end{pmatrix}
= \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
\frac{\partial H}{\partial q_1} \\
\frac{\partial H}{\partial q_2} \\
\frac{\partial H}{\partial p_1} \\
\frac{\partial H}{\partial p_2}
\end{pmatrix}
= \begin{pmatrix}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
-\dot{p}_1 \\
-\dot{p}_2 \\
\dot{q}_1 \\
\dot{q}_2
\end{pmatrix}
\]

This is typically referred to as the matrix or symplectic notation for the Hamilton equations.
Example: Spherical Pendulum

- Pick Generalized Coordinates: $\theta$, $\phi$
- $ds = b d\theta \dot{\theta} + b \sin \theta \ d\phi \dot{\phi}$
- $v = \frac{ds}{dt} = b \dot{\theta} \dot{\theta} + b \sin \theta \dot{\phi} \dot{\phi}$

\[
T = \frac{1}{2} m v^2 = \frac{1}{2} mb^2 \dot{\theta}^2 + \frac{1}{2} mb^2 \sin^2 \theta \dot{\phi}^2 \quad U = -mgb \cos \theta
\]

Thus,

\[
L = T - U = \frac{1}{2} mb^2 \dot{\theta}^2 + \frac{1}{2} mb^2 \sin^2 \theta \dot{\phi}^2 + mgb \cos \theta
\]

E-L equations gives
\[
\begin{align*}
\ddot{\theta} - \dot{\phi}^2 \sin \theta \cos \theta + \frac{g}{b} \sin \theta &= 0 \\
\ddot{\phi} \sin^2 \theta + 2 \dot{\phi} \sin \theta \cos \theta &= 0
\end{align*}
\]
Example: Spherical Pendulum

Practically, we can do one integration immediately through the two constants of motion:

Conservation of $E$:

$$E = \frac{1}{2} mb^2 \dot{\theta}^2 + \frac{1}{2} mb^2 \sin^2 \theta \dot{\phi}^2 - mgb \cos \theta$$

$\phi$ is cyclic, i.e. $\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\phi}} \right) = 0$:

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mb^2 \sin^2 \theta \dot{\phi} = \text{const}$$

These two 1st – order ODEs can be solved easily by substitute $\dot{\phi}$ from the $p_\phi$ equation into the $E$ equation.
Example: Spherical Pendulum

\[ L = \frac{1}{2} m b^2 \dot{\theta}^2 + \frac{1}{2} m b^2 \sin^2 \theta \dot{\phi}^2 + m g b \cos \theta \]

Now, let consider the Hamiltonian Formalism.

We first need to calculate the conjugate momenta:

\[
\begin{align*}
  p_\theta &= \frac{\partial L}{\partial \dot{\theta}} = m b^2 \dot{\theta} \\
  p_\phi &= \frac{\partial L}{\partial \dot{\phi}} = m b^2 \sin^2 \theta \dot{\phi}
\end{align*}
\]

\[
\begin{align*}
  \dot{\theta} &= \frac{p_\theta}{m b^2} \\
  \dot{\phi} &= \frac{p_\phi}{m b^2 \sin^2 \theta}
\end{align*}
\]

The boxed equations are the desired transformation from the config. space to the canonical variables in *phase space*. 
Example: Spherical Pendulum

Construct the Hamiltonian:

\[ H = \dot{q}_j p_j - L \quad (sum) \]

\[ = \dot{\theta} p_\theta + \dot{\phi} p_\phi - L \]

\[ = \frac{p_\theta^2}{mb^2} + \frac{p_\phi^2}{mb^2 \sin^2 \theta} - \frac{1}{2} mb^2 \dot{\theta}^2 - \frac{1}{2} mb^2 \sin^2 \theta \dot{\phi}^2 - mgb \cos \theta \]

\[ = \frac{p_\theta^2}{mb^2} + \frac{p_\phi^2}{mb^2 \sin^2 \theta} - \frac{p_\theta^2}{2mb^2} - \frac{p_\phi^2}{2mb^2 \sin^2 \theta} - mgb \cos \theta \]

\[ H = \frac{p_\theta^2}{2mb^2} + \frac{p_\phi^2}{2mb^2 \sin^2 \theta} - mgb \cos \theta \]

(H is properly expressed in terms of the canonical variables \((\theta, \phi, p_\theta, p_\phi, t)\).)
Example: Spherical Pendulum

Apply Hamilton’s Equations to get four 1st - order ODEs:

\[
\frac{\partial H}{\partial \theta} = -\dot{p}_\theta \quad \Rightarrow \quad \frac{p_\phi^2}{2mb^2}(-2)\sin^{-3}\theta \cos \theta + mb \sin \theta = -\dot{p}_\theta
\]

\[
\dot{p}_\theta = \frac{p_\phi^2 \cos \theta}{mb^2 \sin^3 \theta} - mgb \sin \theta
\]

\[
\frac{\partial H}{\partial \phi} = -\dot{p}_\phi \quad \Rightarrow \quad \dot{p}_\phi = 0
\]

\[
\frac{\partial H}{\partial p_\theta} = \dot{\theta} \quad \Rightarrow \quad \dot{\theta} = \frac{p_\theta}{mb^2}
\]

\[
\frac{\partial H}{\partial p_\phi} = \dot{\phi} \quad \Rightarrow \quad \dot{\phi} = \frac{p_\phi}{mb^2 \sin^2 \theta}
\]

Since \( \phi \) is cyclic, \( P_\phi \) is a constant and \( \phi \) can be integrated to get \( \phi(t) \). We will exploit this later.

Just repeated what we had.
Symmetry and Conservation Theorem Again

- Consider the full-time derivative of $H$,

$$\frac{dH}{dt} = \frac{\partial H}{\partial q_j} \dot{q}_j + \frac{\partial H}{\partial p_j} \dot{p}_j + \frac{\partial H}{\partial t}$$

Using the Hamilton’s Equations:

$$\frac{dH}{dt} = \left(-\dot{p}_j\right)\dot{q}_j + \left(\dot{q}_j\right)p_j + \frac{\partial H}{\partial t}$$

$\Rightarrow \frac{dH}{dt} = \frac{\partial H}{\partial t}$

(soso if time does not explicitly appears in $H$
(time is cyclic), $H$ is conserved!)

Note: $H = E$ if ...

1. $U$ does not depend on the generalized velocities

2. Transformation defining $q_j$ does not depend on $t$

explicitly.
Subtle Difference between $h$ and $H$

Recall that the Jacobi integral $h$ is a function of $(q_j, \dot{q}_j, t)$ instead of $(q_j, p_j, t)$

$$h(q_j, \dot{q}_j, t) = \sum_j \dot{q}_j \frac{\partial L}{\partial \dot{q}_j} - L$$

$$\frac{\partial h}{\partial t} = \sum_j \dot{q}_j \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial t}$$

Also, from the E-L Eq, we know that $-\frac{\partial L}{\partial t} = \frac{dh}{dt}$

Thus, we can rewrite the above equation as,

$$\frac{\partial h}{\partial t} = \sum_j \dot{q}_j \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}_j} \right) + \frac{dh}{dt}$$

Thus, unless the red term is explicitly zero,

$$\frac{\partial h}{\partial t} = 0 \quad \Rightarrow \quad \frac{dh}{dt} = 0$$
Subtle Difference between $h$ and $H$

Example: \[ L = \frac{1}{2} m\dot{q}^2 + \alpha \dot{q} t - V(q) \]

\[ \frac{\partial L}{\partial \dot{q}} = m\dot{q} + \alpha t \]

So,

\[ h = \dot{q} \frac{\partial L}{\partial \dot{q}} - L \]

\[ h = \dot{q}(m\dot{q} + \alpha t) - \left( \frac{1}{2} m\dot{q}^2 + \alpha \dot{q} t - V(q) \right) \]

\[ = m\dot{q}^2 + \alpha \dot{q} q - \frac{1}{2} m\dot{q}^2 - \alpha \dot{q} t + V(q) \]

\[ h = \frac{1}{2} m\dot{q}^2 + V(q) \]
Subtle Difference between $h$ and $H$

$$L = \frac{1}{2} m\dot{q}^2 + \alpha \dot{q} t - V(q) \quad h = \frac{1}{2} m\dot{q}^2 + V(q)$$

So,

$$\frac{\partial L}{\partial t} = \alpha \dot{q} \neq 0 \quad \text{but} \quad \frac{\partial h}{\partial t} = 0$$

From our previous calculations, we have the following relationship,

$$\frac{\partial h}{\partial t} = \dot{q} \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}} \right) + \frac{dh}{dt} = 0$$

So, the LHS is zero and we can also explicitly check that the RHS=0 too but with $\frac{dh}{dt} \neq 0$. 

Subtle Difference between $h$ and $H$

\[
\frac{\partial h}{\partial t} = \dot{q} \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}} \right) + \frac{dh}{dt}
\]

\[
= \dot{q} \frac{\partial}{\partial t} (\alpha t + m\dot{q})
\]

\[
= \alpha \dot{q}
\]

\[
\frac{dh}{dt} = \frac{d}{dt} \left( \frac{1}{2} m\dot{q}^2 + V(q) \right)
\]

\[
= m\ddot{q} \dot{q} + \frac{\partial V}{\partial q} \dot{q}
\]

Thus, we have,

\[
\dot{q} \frac{\partial}{\partial t} \left( \frac{\partial L}{\partial \dot{q}} \right) + \frac{dh}{dt} = \dot{q} \left( m\ddot{q} + \alpha + \frac{\partial V}{\partial q} \right) = 0
\]

This has to be zero since \( \frac{\partial h}{\partial t} = 0 \) and indeed, it does. From EL Eq, we have

\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right) - \frac{\partial L}{\partial q} = 0
\]

\[
\Rightarrow \quad \frac{d}{dt} (\alpha t + m\dot{q}) + \frac{\partial V}{\partial q} = 0
\]

\[
\alpha + m\ddot{q} + \frac{\partial V}{\partial q} = 0
\]
Subtle Difference between $h$ and $H$

$$L = \frac{1}{2}m\dot{q}^2 + \alpha \dot{q}t - V(q) \quad h = \frac{1}{2}m\dot{q}^2 + V(q)$$

So, for this specific example, we have

$$\frac{\partial h}{\partial t} = 0 \quad \text{but} \quad \frac{\partial L}{\partial t} \neq 0 \quad \text{and} \quad \frac{dh}{dt} \neq 0$$

$$= \alpha \dot{q} \neq 0 \quad \text{and} \quad = m\ddot{q} + \frac{\partial V}{\partial q} \dot{q} \neq 0$$

One can also calculate $H(q, p, t)$ using $p \equiv \frac{\partial L}{\partial \dot{q}} = \alpha t + m\dot{q}$

$$H = \frac{(p - \alpha t)^2}{2m} + V(q) \quad \rightarrow \quad \frac{\partial H}{\partial t} = \frac{dH}{dt} \neq 0$$
Symmetry and Conservation Theorem Again

- Other cyclic coordinates:

If \( q_n \) is cyclic, the Lagrangian is \( L = L(q_1, \cdots, q_{n-1}, \dot{q}_1, \cdots, \dot{q}_n, t) \)

The \( n \)-th EOM is then given by:

\[
\frac{\partial L}{\partial \dot{q}_n} = \text{const} \quad \text{(The LHS is usually a complicated function of } q_j \text{ & } \dot{q}_j \text{ and much efforts still needed to solve for } q_n(t).)
\]

In contrast, if \( q_n \) is cyclic in the Hamiltonian Formalism,

\[
\frac{\partial H}{\partial q_n} = 0 = -\dot{p}_n \quad \Rightarrow \quad p_n = \text{const} \quad \text{(conserved)}
\]

(This equation is immediately “solved” from IC \( \rightarrow p_n \) is gone from the prob.)

(The Hamiltonian Formalism has a much nicer structure for cyclic coords)
Routh’s Procedure

**Goal:** Transform only the cyclic coordinates to take advantage of simplicity in phase space for the cyclic variables

Let say we have: \( L = L(q_1, \ldots, q_s, \dot{q}_1, \ldots, \dot{q}_n, t) \) where \( q_{s+1}, \ldots, q_n \) are cyclic

Define the Routhian, \( R = \sum_{j=s+1}^{n} p_j \dot{q}_j - L \) similar to Hamiltonian

where \( R \) depends on \( (q_1, \ldots, q_s, \dot{q}_1, \ldots, \dot{q}_s, p_{s+1}, \ldots, p_n, t) \)

Then, apply the EL equation to non-cyclic variables \((q_1, \ldots, q_s)\),

\[
\frac{d}{dt} \left( \frac{\partial R}{\partial \dot{q}_j} \right) - \frac{\partial R}{\partial q_j} = 0 \quad \text{for} \quad j = 1, \ldots, s
\]

And, apply the Hamilton’s equation to cyclic variables \((q_{s+1}, \ldots, q_n)\)

\[
\frac{\partial R}{\partial q_j} = -\dot{p}_j = 0 \quad \text{and} \quad \frac{\partial R}{\partial p_j} = \dot{q}_j \quad \text{for} \quad j = s + 1, \ldots, n
\]

\((p_j = \text{const})\)
Routh’s Procedure: example

A single particle in a central potential: \( V(r) = -\frac{k}{r^n} \)

From previous chapter, we have: 
\[
L = \frac{m}{2} \dot{r}^2 + \frac{m}{2} r^2 \dot{\theta}^2 + \frac{k}{r^n}
\]

\( \theta \) is cyclic and \( r \) is not, so we define 
\[
p_\theta = \frac{\partial L}{\partial \dot{\theta}} = mr^2 \dot{\theta} \quad \rightarrow \quad \dot{\theta} = \frac{p_\theta}{mr^2}
\]

The Routhian is: 
\[
R = p_\theta \dot{q}_\theta - L
\]

\[
R = \frac{p_\theta^2}{mr^2} - \frac{m}{2} \dot{r}^2 - \frac{m}{2} r^2 \left( \frac{p_\theta}{mr^2} \right)^2 - \frac{k}{r^n} = \frac{p_\theta^2}{2mr^2} - \frac{m}{2} \dot{r}^2 - \frac{k}{r^n}
\]

Depends on \((r, \dot{r}, p_\theta)\) only as advertised
Routh’s Procedure: example

\[ R = \frac{p_\theta^2}{2mr^2} - \frac{m}{2} \dot{r}^2 - \frac{k}{r^n} \]

Applying the EL equation to the non-cyclic variable \( r \) :

\[ \frac{d}{dt} \left( \frac{\partial R}{\partial \dot{r}} \right) - \frac{\partial R}{\partial r} = 0 \quad \Rightarrow \quad -\frac{d}{dt} (\dot{m} \dot{r}) - \left[ \frac{p_\theta^2}{2m} (-2) \frac{1}{r^3} - \frac{k}{r^{n+1}} (-n) \right] = 0 \]

\[ m \ddot{r} - \frac{p_\theta^2}{mr^3} + \frac{nk}{r^{n+1}} = 0 \]

And, the Hamilton’s Equation for \( \theta \) :

\[ \frac{\partial R}{\partial \dot{\theta}} = -\dot{p}_\theta = 0 \quad \frac{\partial R}{\partial p_\theta} = \dot{\theta} = \frac{p_\theta}{mr^2} \]

\[ p_\theta = \text{const} = l \]

\[ \dot{\theta} = \frac{l}{mr^2} \]
Cyclic Variables: Action-Angle Coordinates

- Note that a given system can be described by several different sets of generalized coordinates

  Generalized coordinates are not unique!

- Recall also that the # of cyclic variables can depend on the choice of the generalized coordinates

  e.g., in the previous central force problem:
  → Rect coord \((x, y)\): both \(x, y\) are not cyclic
  → polar coord \((r, \theta)\): \(\theta\) is cyclic
Cyclic Variables: Action-Angle Coordinates

- Although one might not be able to pick a set of generalized coordinates (from a given physical system) to have ALL $q_j$ being cyclic,

  → one can imagine transforming them to an ideal set such that they are all cyclic.

  → **Canonical Transformation** (next Chapter)

- If possible, then,

  → all the conjugate momenta are constant: $p_j = \alpha_j = const$

  → additionally, if $H$ is a constant of motion, then

\[
H = H(\alpha_1, \cdots, \alpha_n) \quad \text{cannot depend on } t \text { and } q_j \text{ explicitly!}
\]
Cyclic Variables: Action-Angle Coordinates

→ consequently, the EOM for the \( q_j \) are simple:

\[
\dot{q}_j = \frac{\partial H}{\partial p_j} = \frac{\partial H}{\partial \alpha_j} = \text{func of cons} \{\alpha_1, \ldots, \alpha_n\} \equiv \omega_j
\]

\[
q_j(t) = \omega_j t + \beta_j
\]

\( \beta_j \) are integration constants depending on IC

- Recall that the “natural” choice of the \( 2n \)-dim phase space variables is with \( q_j \) being the regular generalized coordinates and \( p_j \) being their conjugate momenta.

→ BUT, this is NOT the only choice!

→ The Hamiltonian Formalism can be extended to other possibilities:

\[
Q_j = Q_j(q, p, t) \quad \text{and} \quad P_j = P_j(q, p, t)
\]

(indices for \( q_j, p_j \) are suppressed here)
Cyclic Variables: Action-Angle Coordinates

\[
Q_j = Q_j(q, p, t) \quad \text{and} \quad P_j = P_j(q, p, t)
\]

→ \((Q_j, P_j)\) are the “canonically” transformed variables from the original ones

→ \((Q_j, P_j)\) needs to satisfy the corresponding Hamilton’s Equations in the transformed coordinates.

→ There are no preference between the transformation above for \(Q_j \& P_j\)

The canonical transformation treats both \(Q_j \& P_j\) equally.

→ \(Q_j \& P_j\) are on the same theoretical footing in the Hamiltonian Formalism!

→ The Hamiltonian Formalism is the starting point in analyzing QM systems.
Connection to Statistical Mechanics

- The Hamilton’s Equations describe motion in **phase space**
- A point in phase space \((q_j, p_j)\) uniquely determines the state of the system AND its future evolution.
- Nearby points represent system states with similar but slightly different initial conditions.
- One can imagine a *cloud of points* bounded by a closed surface \(S\) with nearly identical initial conditions moving in time.
Connection to Statistical Mechanics

- Let say at time $t$, a small subset of these points crosses a differential area $da$ on $S$ in a given outward normal direction $\hat{n}$ such that $da = da\hat{n}$

- Let $v = \left(\langle \dot{q}_j \rangle, \langle \dot{p}_j \rangle \right)$ be the mean “velocity” for points in $da$

- Then, after a given time $dt$, this small subset of points will trace out a differential volume in phase space given by

$$vdtda$$
Connection to Statistical Mechanics

- Summing up all points in the cloud bounded by $S$, we have,

$$
\frac{dV}{dt} = \left( \oint_S \mathbf{v} \cdot d\mathbf{a} \right) dt
$$

or,

$$
\frac{dV}{dt} = \oint_S \mathbf{v} \cdot d\mathbf{a}
$$

rate of change of “phase-space volume” due to the motion of the points

- Then, by Gauss’s Law, we have

$$
\frac{dV}{dt} = \oint_S \mathbf{v} \cdot d\mathbf{a} = \int_V (\nabla \cdot \mathbf{v}) dV
$$

$V$ enclosed by $S$
Liouville’s Theorem

\[
\frac{dV}{dt} = \oint_S \mathbf{v} \cdot d\mathbf{a} = \int_V (\nabla \cdot \mathbf{v}) dV
\]

- In phase space, we have \( \mathbf{v} = (\dot{q}_1 \hat{q}_1 + \cdots + \dot{q}_n \hat{q}_n + \dot{p}_1 \hat{p}_1 + \cdots + \dot{p}_n \hat{p}_n) \)

- So that,

\[
\int_V (\nabla \cdot \mathbf{v}) dV = \int_V \sum_k \left( \frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k} \right) dV \quad (*)
\]

- Using the Hamilton’s Equations, we have:

\[
\frac{\partial \dot{q}_k}{\partial q_k} = \frac{\partial}{\partial q_k} \left( \frac{\partial H}{\partial p_k} \right) = \frac{\partial^2 H}{\partial q_k \partial p_k}
\]

\[
\frac{\partial \dot{p}_k}{\partial p_k} = \frac{\partial}{\partial p_k} \left( - \frac{\partial H}{\partial q_k} \right) = - \frac{\partial^2 H}{\partial p_k \partial q_k}
\]
Liouville’s Theorem

- Substituting into Eq (*), we have,

\[
\frac{dV}{dt} = \int \sum_{k} \left( \frac{\partial^2 H}{\partial q_k \partial p_k} - \frac{\partial^2 H}{\partial p_k \partial q_k} \right) dV
\]

\[ (H \text{ is a smooth function}) \]

\[
\frac{dV}{dt} = 0!
\]

This is the Liouville’s Theorem: collection of phase-space points move as an incompressible fluid.

→ Phase space volume occupied by a set of points in phase space is constant in time.
Liouville’s Theorem

This is the starting point for statistical mechanics

- Imagine many \((N)\) identical mechanical systems but with different initial conditions (ensemble of systems).
- Each is a different point in phase space with \((q_j, p_j)\)
- Statistical properties can be specified by a “density of states” function per unit volume in phase space

\[
\rho(q_j, p_j, t) dV = \# \text{ system points in phase space volume } dV \text{ located at } (q_j, p_j) \text{ at time } t.
\]
Liouville’s Theorem

At statistical equilibrium,

→ The # of points in the ensemble \((N)\) does not change

→ Then, since \(N\) is fixed, \(V\) stays constant, \(\rho = N/V = \text{constant as well!}\)

Thus, Liouville’s Thm implies: density \(\rho\) in a neighborhood of any system state = const as the system evolves in phase space.

→ Thus, equilibrium \(\rho\) is uniform along the flow lines of the system points. (SM’s Master Eq. or Fokker-Planck Eq.)

→ This condition is typically used to solve for the equilibrium distribution \(\rho_{eq}\) for a statistical mechanical problem in phase space with which various statistical averages, \(P, T, U, S,...\) can be calculated.