Hamilton's equations:

Start with a Lagrangian $L$

Lagrange's eqs. are
\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \]

Now introduce canonical momentum
\[ p_i = \frac{\partial L}{\partial \dot{q}_i} \]

Then the Lagrange's equations become
\[ \dot{p}_i = \frac{\partial L}{\partial q_i} \]

We are now going to express our eqs.
of motion not in terms of $L(\dot{q}_i, \ddot{q}_i, t)$, but rather in terms of another function of variables $\dot{q}_i, \ddot{q}_i, t$.

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

where $L = L(\dot{q}_i, \ddot{q}_i, t)$ (sums over $i$ implied)
Now introduce 
\[ H = \dot{q}_i \dot{p}_i - L \]

This is an example of a Legendre transformation (see below). Then 
\[ \Delta H = \dot{q}_i \Delta p_i + \dot{p}_i \Delta q_i - \frac{\partial L}{\partial \dot{q}_i} \Delta q_i - \frac{\partial L}{\partial q_i} \Delta \dot{q}_i - \frac{\partial L}{\partial \dot{p}_i} \Delta \dot{p}_i - \frac{\partial L}{\partial \dot{p}_i} \Delta p_i \]

\[ = \dot{q}_i \Delta p_i - \frac{\partial L}{\partial q_i} \Delta \dot{q}_i - \frac{\partial L}{\partial \dot{p}_i} \Delta \dot{p}_i \]

This shows that 
\[ \frac{\partial H}{\partial \dot{p}_i} = \dot{q}_i ; \quad \frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i} = -\dot{p}_i ; \quad \frac{\partial H}{\partial \dot{q}_i} = -\frac{\partial L}{\partial \dot{q}_i} \]

or, collecting terms
\[ \begin{align*}
\dot{q}_i &= \frac{\partial H}{\partial \dot{p}_i} \\
\dot{p}_i &= -\frac{\partial H}{\partial q_i} \\
-\frac{\partial L}{\partial \dot{q}_i} &= \frac{\partial H}{\partial \dot{q}_i}
\end{align*} \]

"Hamilton's equations"

2n + 1 1st order equations

rather than n second order and one first order Lagrange eqs.
where \( H = \Pi \dot{q} - L \)

Simple example:
\[
L = \frac{1}{2} m \dot{q}^2 - V(q)
\]
\[
H = \Pi \dot{q} - L = \frac{\partial L}{\partial \dot{q}} \hat{q} - L = (m \dot{q}) \dot{q} - L
\]
\[
= m \dot{q}^2 - \frac{1}{2} m \dot{q}^2 + V(q)
\]
\[
= \frac{1}{2} m \dot{q}^2 + V(q)
\]

But \( \Pi = \frac{\partial L}{\partial \dot{q}} = m \dot{q} \)

So \( H = \frac{\Pi^2}{2m} + V(q) \)

Hamilton's equations become
\[
\dot{q} = \frac{\partial H}{\partial \Pi} = \frac{\Pi}{m}
\]
\[
\dot{\Pi} = -\frac{\partial H}{\partial q} = -\frac{\partial V}{\partial q}
\]

or \( m \dot{q}^2 = -\frac{\partial V}{\partial q} \) (same as Lagrangian equation)

There is a broad range of cases where \( L = T - V \)
and \( H = T + V \), namely, if \( L \) is a quadratic function of the generalized velocities.
\[ L = \frac{1}{2} \sum_{i} \sum_{j} \left( \dot{x}_i \dot{x}_j \right) - V(\mathbf{x}) \]

\[ p_i = \sum_{j} L_{ij}(\mathbf{\dot{x}}) \dot{x}_j \]

\[ H = p_i \dot{x}_i - L \]

\[ = \sum_{i} L_{ij}(\mathbf{\dot{x}}) \dot{x}_i - V(\mathbf{x}) L \]

\[ = T + V \quad \text{assuming } L \text{ is independent of time} \]

Another example:

\[ L = \frac{1}{2} m \left( \dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right) - V(x, y, z) \]

\[ p_x = m \dot{x}, \quad p_y = m \dot{y}, \quad p_z = m \dot{z} \]

\[ \Rightarrow H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) \]

All charged particles in an electromagnetic field:

\[ L = T - V = \frac{1}{2} m \dot{x}_i^2 + q \phi + q A_i \dot{x}_i \]

\[ = \frac{1}{2} m \dot{x}_i \dot{x}_i - q \phi + q A_i \dot{x}_i \]

\[ p_i = \frac{\partial L}{\partial \dot{x}_i} = m \dot{x}_i + q A_i \]

\[ \text{Another example:} \]

\[ L = \frac{1}{2} m \left( \dot{x}^2 + \dot{y}^2 + \dot{z}^2 \right) - V(x, y, z) \]

\[ p_x = m \dot{x}, \quad p_y = m \dot{y}, \quad p_z = m \dot{z} \]

\[ \Rightarrow H = \frac{p_x^2 + p_y^2 + p_z^2}{2m} + V(x, y, z) \]

\[ \text{All charged particles in an electromagnetic field:} \]

\[ L = T - V = \frac{1}{2} m \dot{x}_i^2 + q \phi + q A_i \dot{x}_i \]

\[ = \frac{1}{2} m \dot{x}_i \dot{x}_i - q \phi + q A_i \dot{x}_i \]

\[ p_i = \frac{\partial L}{\partial \dot{x}_i} = m \dot{x}_i + q A_i \]
Then \( m \dot{v}_i = p_i - q A_i \) and

\[
H = p_i \dot{v}_i - L
\]

\[
= p_i \left( \frac{p_i - q A_i}{m} \right) - \frac{1}{2} m \left( \frac{p_i - q A_i}{m} \right) \left( \frac{p_i - q A_i}{m} \right)
+ q \phi - q A_i \left( \frac{p_i - q A_i}{m} \right)
\]

\[
= \left( \frac{p_i - q A_i}{m} \right) \left( \frac{p_i - q A_i}{m} \right) + q \phi
\]

\[
= \frac{1}{2} \left( p - q A \right) \left( p - q A \right) + q \phi
\]

These are guaranteed to give the same eqs. of motion as \( L \).

Another general example (see book):

\[
L \left( E_{ik}, \dot{E}_{ik}, t \right) = L_0 \left( E_{ik}, t \right)
+ \frac{1}{2} \epsilon_{ijk} \dot{E}_{ik} \dot{E}_{ij}
+ a_i \left( \dot{E}_{ik}, t \right) \dot{q}_i + T_{ij} \left( \dot{E}_{ik}, t \right) \dot{q}_i \dot{q}_j
\]

See book: \( p_i = T_{ij} \dot{q}_j + a_i \)

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

\[
= \frac{1}{2} \left( p - a \right) \left( T^{-1} \right)_{ij} \left( p - a \right)_j - L_0 \left( E_{ik}, t \right)
\]
Another example: single particle in spherical coordinates

\[ L = \frac{m v^2}{2} = - V \]

\[ = \frac{1}{2} m \left( r^2 + r^2 \sin^2 \theta \phi^2 + r^2 \dot{\theta}^2 \right) - V(r, \theta, \phi) \]

\[ p_r = m \dot{r} \quad p_\phi = m r^2 \sin^2 \theta \dot{\phi} \]
\[ p_\theta = m r^2 \dot{\theta} \]

Plug back in and get

\[ H = T + V = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2 \theta} + V(r, \theta, \phi) \]

If \( L \) does not depend on time

(and hence \( H \) does not depend on time explicitly)

then \( H \) is a const. of the motion.

Proof:

\[ \frac{dH}{dt} = \frac{\partial H}{\partial t} + \frac{\partial H}{\partial p_i} \dot{p}_i + \frac{\partial H}{\partial q_i} \dot{q}_i \]

\[ = - \frac{\partial H}{\partial t} - \frac{\partial H}{\partial p_i} \frac{\partial H}{\partial q_i} + \frac{\partial H}{\partial q_i} \frac{\partial H}{\partial p_i} = 0 \]

if \( \frac{\partial H}{\partial t} = 0 \)
If \( q_i \) is absent from \( H \) then
\[
\dot{q}_i = -\frac{\partial H}{\partial \dot{q}_i} = 0 \Rightarrow \dot{q}_i = \text{const. of motion}
\]

(If \( q_i \) is cyclic)

Since if \( H \) does not depend on \( q_i \), this means that there is some symmetry in problem

E.g. If \( V(p) = V(r) \) only, then
\[
P_\theta = m r^2 \dot{\theta} \neq \text{const.}
\]

and \( P_\phi = m r^2 \sin^2 \theta \dot{\phi} = \text{const.} \)

= \( z \)-component of angular momentum

---

Poisson brackets:

\[
\{u, v\}_{p, q} = \sum_{i=1}^{n} \left( \frac{\partial u}{\partial q_i} \frac{\partial v}{\partial p_i} - \frac{\partial u}{\partial p_i} \frac{\partial v}{\partial q_i} \right)
\]

Note that:

\[
\{p_k, p_l\}_{q, p} = 0
\]

\[
= \frac{\partial p_k}{\partial q_i} \frac{\partial p_l}{\partial p_i} - \frac{\partial p_k}{\partial p_i} \frac{\partial p_l}{\partial q_i} = 0
\]

(Causing Poisson summation convention)

Similarly \( \{q_k, q_l\}_{q, p} = 0 \)

But \( \{q_k, p_l\}_{q, p} = \delta_{kl} = -\{p_k, q_l\}_{q, p} \)
Rather similar (in form) to commutator brackets.

Also,

\[
\frac{du}{dt} = \frac{\partial u}{\partial \mathbf{v}} \frac{d\mathbf{v}}{dt} u(\mathbf{v}(t), \mathbf{q}(t), t)
\]

\[
= \frac{\partial u}{\partial t} + [u, H]
\]

\[
\text{Proof:}
\]

\[
\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial \mathbf{v}_i} \mathbf{v}_i + \frac{\partial u}{\partial \mathbf{q}_i} \mathbf{q}_i
\]

\[
= \frac{\partial u}{\partial t} + \frac{\partial u}{\partial \mathbf{v}_i} \frac{\partial H}{\partial \mathbf{q}_i} + \frac{\partial u}{\partial \mathbf{q}_i} \frac{\partial H}{\partial \mathbf{v}_i}
\]

\[
= \frac{\partial u}{\partial t} + [u, H] \quad \text{QED}
\]

(again, similar to operator eqs. of motion in quantum mechanics)
Application of Hamilton's eqs. of motion

Long collection of springs connected to masses:

\[ L = \frac{k}{2} \sum_{n=1}^{N} (\eta_{n+1} - \eta_n)^2 + \frac{m}{2} \sum_{n} \dot{\eta}_n^2 \]

\( p_n = m \dot{\eta}_n \); by our general principle

\[ H = \sum_{n} \frac{p_n^2}{2m} + \frac{k}{2} \sum_{n} (\eta_{n+1} - \eta_n)^2 \]

Eq. of motion \( \dot{p}_n = \frac{\partial H}{\partial \eta_n} = k \left( \eta_{n+1} - 2\eta_n + \eta_{n-1} \right) \)

\[ \dot{p}_n = k \eta_n \]

Same as obtained from Lagrange eqs. of motion
Driven small oscillations:

(a) Single oscillator:

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} k x^2 + x F(t)$$

Then eq. of motion is

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = 0 \quad \text{or} \quad m \ddot{x} + k x - F(t) = 0$$

Simplest case: $F(t)$ is monochromatic

$$F(t) = F_0 \cos \omega t = \text{Re} (F_0 e^{-i \omega t})$$

(taking $F_0$ to be real).

Then look for a particular solution of the form

$$x(t) = \text{Re} \left[ x_0 e^{-i \omega t} \right]$$

So

$$\text{Re} \left[ -i \omega x_0 e^{-i \omega t} + k x_0 e^{-i \omega t} \right] = \text{Re} \left[ F_0 e^{-i \omega t} \right]$$

or in general, dropping "Re",

$$(-i \omega x_0 + k x_0) = F_0$$

$$x_0 = \frac{F_0}{k - \omega^2 m} = \frac{F_0}{\omega_0^2 - \omega^2} \quad \text{where} \quad \omega_0 = \frac{k}{m}$$

$$x(t) = \text{Re} \left[ \frac{F_0}{\omega_0^2 - \omega^2} e^{-i \omega t} \right] \to \infty \quad \text{as} \quad \omega \to \pm \omega_0$$
This is the well-known phenomenon of resonance: large response when applied force is near frequency of natural oscillations.

What if $F(t)$ is not a monochromatic field?

The most straightforward way to solve the eq. of motion in this case is by Fourier transform. However, there is another way to do it. Rewrite the equation of motion as

$$\dot{x} + \omega_0^2 x = F(t)/m$$

Now define $\xi = \dot{x} + i\omega_0 x$ (which is complex)

Then the eq. of motion becomes

$$\ddot{\xi} - i\omega_0 \dot{\xi} = F(t)/m$$

$$= \dot{x} + i\omega_0 \dot{x} - i\omega_0 \dot{x} + \omega_0^2 x = \dot{x} + \omega_0^2 x$$

Try a solution of the form

$$\xi(t) = A(t) e^{i\omega_0 t} \quad (\text{This solves homogeneous eq. if } F = 0)$$

$$\Rightarrow A e^{i\omega_0 t} + i\omega_0 A e^{i\omega_0 t} - i\omega_0 A e^{i\omega_0 t} = F(t)/m$$

$$A = e^{-i\omega_0 t} F(t)/m$$

$$A(t) = A(0) + \int_0^t e^{-i\omega_0 t'} F(t') dt'$$
and thus

\[
\xi(t) = e^{i\omega_0 t} \left[ \int_0^t \frac{1}{m} F(t') e^{-i\omega_0 t'} dt' + \xi_0 \right]
\]

where \( \xi_0 = A(0) \)

and \( x(t) = \frac{1}{\omega_0} \text{Im} \xi(t) \)

This is the general solution for an arbitrary forcing term.

Total energy absorbed. Suppose we start at \( t = -\infty \) with \( \xi_0 = A(-\infty) = 0 \). Then \( \xi(t) \) is

\[
\xi(t) = \frac{1}{m} e^{i\omega_0 t} \int_{-\infty}^t \frac{1}{m} F(t') e^{-i\omega_0 t'} dt'
\]

with \( t \to +\infty \)

Then \( |\xi(t)|^2 = \frac{1}{m^2} \int_{-\infty}^{\infty} e^{-i\omega_0 t'} F(t') dt' \)

The total energy of the oscillator is:

\[
E = \frac{1}{2} m \left( \dot{x}^2 + \frac{1}{2} \omega^2 x^2 \right)
\]

\[
= \frac{1}{2} m |\xi|^2 \quad \text{since} \quad \xi = x + i\omega_0 x
\]

So \( |\xi|^2 = |x|^2 + \omega_0^2 x^2 \)

\[
\Rightarrow E = \frac{1}{2m} \left| \int_{-\infty}^{\infty} e^{-i\omega_0 t'} F(t') dt' \right|^2
\]
Examples: (all with $x(0) = \dot{x}(0) = 0$

(a) $F(t) = \text{const.} = F_0$

Then $\xi(t) = e^{i\omega_0 t} \int_0^t \frac{F_0}{m} e^{-i\omega_0 t'} dt'$

$= e^{i\omega_0 t} \frac{F_0}{m} \left[ e^{-i\omega_0 t'} - 1 \right] / (-i\omega_0)$

$= \frac{F_0}{m} \left( 1 - e^{i\omega_0 t} \right) / (-i\omega_0) = \frac{iF_0}{m\omega_0} (1 - e^{i\omega_0 t})$

$x(t) = \frac{1}{\omega_0} \text{Im } \xi(t) = \frac{F_0}{m\omega_0} (1 - \cos \omega_0 t)$

(This is just a damped harmonic oscillator)

(b) $F = at$

$\xi(t) = e^{i\omega_0 t} \int_0^t \frac{at'}{m} e^{-i\omega_0 t'} dt'$

Need to integrate $\int_0^t e^{-i\omega_0 t'} dt'$

$= \left[ \frac{t'}{-i\omega_0} e^{-i\omega_0 t'} \right]_0^t - \int_0^t \frac{1}{(-i\omega_0)} \left( -i\omega_0 e^{-i\omega_0 t'} \right) dt'$

and after simplification, one obtains

$x(t) = \frac{a}{m\omega_0^2} (\omega_0 t - \sin \omega_0 t)$
(c) \[ F = F_0 \exp(-\alpha t) \]

This gives:

\[ x(t) = \frac{F_0}{\omega_0^2 + \alpha^2} \left[ \exp(-\alpha t) \left( \cos \omega_0 t + \frac{\alpha}{\omega_0} \sin \omega_0 t \right) \right] \]

(d) \[ F = F_0 \exp(-\alpha t) \cos \beta t \]

Here one finds:

\[ x = \frac{F_0}{\omega_0^2 + \alpha^2 - \beta^2} K_1(t) / K_2(t) \]

where \[ K_1(t) = \left( \frac{\omega_0}{\omega_0^2 + \alpha^2 - \beta^2} \right) \cos \omega_0 t \]

\[ + \frac{\alpha}{\omega_0} \left( \omega_0^2 + \alpha^2 - \beta^2 \right) \sin \omega_0 t + \exp(-\alpha t) \left( \omega_0^2 + \alpha^2 - \beta^2 \right) \cos \beta t - 2\alpha \beta \sin \beta t \]

\[ K_2(t) = m \left( \frac{\omega_0}{\omega_0^2 + \alpha^2 - \beta^2} \right)^2 + 4\alpha^2 \beta^2 \]

This case is best treated by writing the force in the complex form:

\[ F = F_0 \exp \left[ (-\alpha + i\beta) t \right] \]

and taking the real part as needed.

Try these as optional exercises.
Dissipation:

Suppose we just have a periodic external force $f \cos \omega t$ and a frictional force of the form $-\alpha x$. Then we have

$$m \ddot{x} = -m \omega_0^2 x - \dot{x} + f \cos \omega t$$

or

$$\ddot{x} + \frac{\alpha}{m} \dot{x} + \omega_0^2 x = \frac{f}{m} \cos \omega t = \text{Re} \left( \frac{f}{m} e^{i \omega t} \right)$$

Easiest done using complex notation, as above

Write $x = \text{Re} \left[ B e^{i \omega t} \right]$.

Then

$$(-\omega^2 + i \frac{\alpha}{m} \omega + \omega_0^2) B = \frac{f}{m}$$

So

$$B = \frac{f/m}{-\omega^2 + i \frac{\alpha}{m} \omega + \omega_0^2} = \frac{f}{\omega_0^2 + \frac{\alpha}{m} \omega - \omega^2}$$

$$\omega_0^2 + \frac{\alpha}{m} \omega - \omega^2 = \omega_0^2 \frac{m}{m} (\omega_0^2 - \omega^2 + 2i \lambda \omega)$$

where $2 \lambda = \frac{\alpha}{m}$

We can write $B = b e^{i \delta}$

$$b = \frac{f/m}{\sqrt{(\omega_0^2 - \omega^2)^2 + 4 \lambda^2 \omega^2}}$$

$$\tan \delta = \frac{2 \lambda \omega}{\omega^2 - \omega_0^2}$$
The general form of the solution is thus
\[ x(t) = b \cos(\omega t + \delta) \]

E.g. suppose \( \lambda \ll \omega \).

Mean-squared amplitude \( b^2 \):

\[ b^2 \]

Phase angle \( \delta \):

What about the driven oscillations in systems with
systems of oscillators:

\[ \text{E.g., } \begin{array}{ccc} 1 & 2 & 3 \\ m & M & m \end{array} \]

\[ L = \frac{1}{2} \left[ m (\ddot{\eta}_1 + \ddot{\eta}_3)^2 + M \dot{\eta}_2^2 \right] - \frac{k}{2} \left[ (\eta_2 - \eta_1)^2 + (\eta_3 - \eta_2)^2 \right] \]

The equations of motion, as already shown, are

\[ m \ddot{\eta}_1 = k (\eta_2 - \eta_1) = -m \omega^2 \eta_1 \]
\[ m \ddot{\eta}_3 = k (\eta_2 - \eta_3) = -m \omega^2 \eta_3 \]
\[ M \ddot{\eta}_2 = k (\eta_3 - 2\eta_2 + \eta_1) = -M \omega^2 \eta_2 \]

The frequencies are thus determined by the equation

\[ \det \begin{vmatrix} k - m \omega^2 & -k & 0 \\ -k & 2k - M \omega^2 & -k \\ 0 & -k & k - m \omega^2 \end{vmatrix} = 0 \]

or

\[ (k - m \omega^2)^2 (2k - M \omega^2) - 2k^2 (k - m \omega^2) = 0 \]

and there are corresponding eigenvectors

for each of the three allowed frequencies (including \( \omega = 0 \)).
Now let's imagine that this molecule is driven by an applied electric field \( \mathbf{E} = E_0 \mathbf{e}_x \cos \omega t \). We assume that the mass \( M \) has charge \( 2q \), and that the other two masses each have charge \(-q\). Then our equations of motion are:

\[
\begin{align*}
\ddot{\eta}_1 &= k(\eta_2 - \eta_1) + qE_0 e^{-i\omega t} = -m_0^2 \eta_1 \\
\ddot{\eta}_2 &= k(\eta_3 - 2\eta_2 + \eta_1) + 2qE_0 e^{i\omega t} = -m_0^2 \eta_2 \\
\ddot{\eta}_3 &= k(\eta_2 - \eta_3 - qE_0 e^{-i\omega t}) = -m_0^2 \eta_3
\end{align*}
\]

or:

\[
\begin{pmatrix}
k - m_0^2 & -k & 0 \\
-k & 2k - M_0^2 & -k \\
0 & -k & k - m_0^2
\end{pmatrix}
\begin{pmatrix}
\eta_1 \\
\eta_2 \\
\eta_3
\end{pmatrix}
= qE_0
\begin{pmatrix}
-1 \\
2 \\
-1
\end{pmatrix}
\]

Thus:

\[
\begin{pmatrix}
\eta_1 \\
\eta_2 \\
\eta_3
\end{pmatrix}
= \begin{pmatrix}
k - m_0^2 & -k & 0 \\
-k & 2k - M_0^2 & -k \\
0 & -k & k - m_0^2
\end{pmatrix}^{-1}
\begin{pmatrix}
-qE_0 \\
2qE_0 \\
-qE_0
\end{pmatrix}
\]

So it appears that we will get a very strong response whenever the frequency of the applied field coincides with a natural mode of oscillation of the system. However, the perturbation may not actually drive all of the molecules, i.e.
it may not couple to all the normal modes. For example, in the case of the three-atom molecule, the electric field will not couple to the zero-frequency mode because the molecule has no net charge and hence will not be moved by this a static electric field.

As shown previously, there are three modes:

\[ w_1 = 0, \quad w_2 = \sqrt{\frac{k}{m}}, \quad w_3 = \sqrt{\frac{k}{m}(1 + \frac{2m}{M})} \]

and, with \( \eta_i = a_i e^{-i\omega t} \),

\[ w = w_1, \quad a_1 = a_2 = a_3 \]

\[ w = w_2, \quad a_1 = -a_3, \quad a_2 = 0 \]

\[ w = w_3, \quad a_1 = a_3 = \frac{1}{\sqrt{2m(1 + \frac{2m}{M})}}, \quad a_2 = -\frac{2}{\sqrt{2m(2 + \frac{M}{m})}} \]

Of the three modes, \( w_2 \) does not couple to the electric field and there is no singular response near \( w_2 \).

There is however a strong response which becomes singular near \( w = w_3 \).

If there is damping, there will be a strong absorption near \( w = w_3 \) which can be calculated using

\[ P = \text{power absorbed} = \sum_{i=1}^{3} \left\langle \vec{F}_i \cdot \vec{\eta}_i \right\rangle \]