1) Conservation of angular momentum in Hamiltonian mechanics: A particle moves in three dimensions and its state is specified by the position $\mathbf{q}$ and the momentum $\mathbf{p}$. Under an infinitesimal rotation of the state, $\mathbf{q}$ and $\mathbf{p}$ transform according to:

$$\begin{aligned}\mathbf{q} &\to \mathbf{q} + \delta\mathbf{q} = \mathbf{q} + \mathbf{a}\times\mathbf{q} \\ \mathbf{p} &\to \mathbf{p} + \delta\mathbf{p} = \mathbf{p} + \mathbf{a}\times\mathbf{p}\end{aligned}$$

where $\mathbf{a}$ is a vector of infinitesimal magnitude describing a rotation through angle $|\mathbf{a}|$ about the axis specified by $\mathbf{a}/|\mathbf{a}|$.

a) Show that $G \equiv \mathbf{a}\cdot(\mathbf{q}\times\mathbf{p})$ is the generator of this infinitesimal transformation, and that the transformation is canonical.

b) Consider the hamiltonian

$$\mathcal{H} = \frac{1}{2m}|\mathbf{p}|^2 + U(|\mathbf{q}|).$$

Show that the Poisson bracket $\{\mathcal{H}, G\}$ vanishes for arbitrary infinitesimal $\mathbf{a}$, and hence that angular momentum is conserved.

c) The angular momentum vector $\mathbf{L}$ has cartesian components L_μ (with $\mu = 1, 2, 3$). Evaluate the Poisson brackets $\{L_\mu, L_\nu\}$ between them. Explain why the transformation to a pair of components of angular momentum cannot be a canonical transformation.

2) Hamiltonian mechanics and Poisson brackets – only parts (g) to (l) are mandatory: As Hamilton discovered, there are significant virtues associated with making yet another reformulation of mechanics, beyond the *Newton* $\Rightarrow$ *Lagrange* $\Rightarrow$ *Stationary Action* reformulations that we have already encountered. Amongst these virtues are: a set of dynamical equations – the so-called canonical equations – that is even more simple and symmetrical in its structure than Lagrange's equations; the freedom to make transformations not only between convenient sets of generalised coordinates, but also to make so-called canonical transformations, *i.e.*, transformations that mix the generalised momenta and coordinates under which the canonical equations retain their form (thus breaking the link between coordinates and velocities that is inherent in the Lagrangian framework); and a formulation for classical mechanics that provides the most straightforward platform from which to embark upon quantum mechanics. In Hamilton's formulation the coordinates and momenta appear on what is an essentially equal footing.

Recall that in the Lagrangian formulation of mechanics we focus on the generalised coordinates $\{q_j\}_{j=1}^n$ and the associated generalised velocities $\{\dot{q}_j\}_{j=1}^n$. In particular, the dynamics is governed by the Lagrangian function L, which is a function of the generalised coordinates, the generalised velocities and, possibly, the time.

Hamilton discovered that it is possible to reformulate dynamics so as to eliminate all reference to the generalised velocities, focusing instead on the generalised momenta $\{p_j\}_{j=1}^{n}$. Recall that the generalised momenta have thus far been defined as functions depending on the generalised coordinates and momenta and possibly the time: $p_j \equiv \partial L/\partial \dot{q}_j$ (for $j = 1, \ldots n$). By contrast, in Hamilton's formulation one specifies the state of the system not by the coordinates and velocities but instead by the coordinates and momenta. This formulation is called hamiltonian mechanics or, sometimes, the canonical formulation (canonical meaning appointed by canon law, included in canon scripture, authoritative or accepted).

The primary question is this: what is the form of the equations of motion that govern the generalised coordinates and momenta? The answer is found by making a Legendre transformation that exchanges the generalised velocities for generalised momenta. We shall address this issue for a system described by a single generalised coordinate, and then extend the results to a system with several degrees of freedom.

a) Consider a dynamical system specified by the Lagrangian $L(q, \dot{q}, t)$. By considering a small variation in L and using the Euler-Lagrange equation, show that the hamiltonian obtained through the Legendre transformation $H = p\dot{q} - L$ is a function of q, p and t.

b) By identifying the coefficients of the variation of H, construct Hamilton's equations of motion. (It is crucial to understand that the independent variables are now q, p and t, and not q, $\dot{q}$ and t.) The dynamics of the system is now specified by the hamiltonian $H(q, p, t)$ rather than the Lagrangian $L(q, \dot{q}, t)$. There are now two (typically coupled) first order differential equations of motion (Hamilton's equations), rather than one second order equation of motion (the Euler-Lagrange equation).

c) Generalise parts (a) and (b) to the case of a system with n degrees of freedom. How many hamiltonian equations of motion do you find?

d) Consider a free particle with Lagrangian $L = m\dot{q}^2/2$. Construct the hamiltonian and, hence, Hamilton's equations of motion. Solve Hamilton's equations.

e) Consider the harmonic oscillator with Lagrangian $L = m\dot{q}^2/2 - kq^2/2$. Construct the hamiltonian and, hence, Hamilton's equations of motion. Solve Hamilton's equations of motion. (You would be correct to observe that solving Hamilton's equations is neither easier nor harder than solving the Euler-Lagrange equation. The advantages of the hamiltonian formulation are associated with the structure of the theory and the freedom to choose from a much wider class of independent variables. Furthermore, quantum mechanics is most readily formulated starting from the hamiltonian view.)

f) Show that, by virtue of Hamilton's equations, $dH/dt = \partial H/\partial t$. (Note: this shows that the hamiltonian is conserved if it does not explicitly depend on time.)

Consider a system with one pair of canonically conjugate variables, q and p. Then introduce a pair of functions $A(q, p, t)$ and $B(q, p, t)$. (Such functions are called *functions on phase space*.) Poisson discovered that it can be useful to introduce a new function on phase space, derived from A and B, called the Poisson bracket of A and B. The Poisson bracket is denoted by $\{A, B\}$ and is defined as follows:

$$\{A, B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}.$$

g) Compute the so-called fundamental Poisson bracket $\{q, p\}$.

h) Compute the following Poisson brackets:

(h.i) $\{q, q\}$

(h.ii) $\{p, p\}$

(h.iii) $\{p^2, q\}$

(h.iv) $\{V(q), p\}$

j) Show that any function on phase space C evolves in time according to the Poisson equation of motion

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + \{C, H\}.$$

Notice that the Poisson bracket of C with the hamiltonian thus gives us an efficient method for testing whether C is conserved.

k) Write Hamilton's equations using Poisson brackets.

We now consider the case of several degrees of freedom. In the Lagrangian description we have a collection of generalised coordinates and velocities, $\{q_j\}_{j=1}^n$ and $\{\dot{q}_j\}_{j=1}^n$, and a Lagrangian function L that depends on these coordinates and velocities and, possibly, the time. The transformation to the hamiltonian point of view proceeds along the following lines:

- Construct the generalised momenta $\{p_j\}_{j=1}^n$ using $p_j = \partial L/\partial \dot{q}_j$. The momentum p_j is called the momentum canonically conjugate to the coordinate q_j. The pairs $\{(q_j, p_j)\}_{j=1}^n$ are said to form canonically conjugate pairs of coordinates and momenta.
- Construct the hamiltonian, a function of the coordinates and momenta, through the Legendre transformation

$$H(\{q_j\}_{j=1}^n, \{p_j\}_{j=1}^n, t) = \sum_{k=1}^{n} \dot{q}_k p_k - L(\{q_j\}_{j=1}^n, \{\dot{q}_j\}_{j=1}^n, t).$$

- Then Hamilton's equations become

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} \qquad \text{and} \qquad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j} \qquad \text{for} \quad j = 1, \ldots, n.$$

l) Construct the hamiltonian and solve Hamilton's equations for the following systems:

(l.i)] a free particle moving in three dimensions, for which the Lagrangian is given by $L = m|\dot{\mathbf{r}}|^2/2$

(l.ii) a three dimensional harmonic oscillator, for which the Lagrangian is given by $L = m|\dot{\mathbf{r}}|^2/2 - k|\mathbf{r}|^2/2$

For systems with several degrees of freedom the Poisson bracket is defined to be

$$\{A, B\} = \sum_{k=1}^{n} \left(\frac{\partial A}{\partial q_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial q_k} \right).$$

m) For a single particle moving in three dimensions compute the following Poisson brackets:

(m.i) the fundamental Poisson brackets $\{q_i, p_j\}$

(m.ii) the Cartesian components of the angular momentum $\mathbf{L} = \mathbf{q} \times \mathbf{p}$, *i.e.*, $\{L_i, L_j\}$

(m.iii) the Cartesian components of the angular momentum with the squared magnitude of the angular momentum, *i.e.*, $\{L_i, L^2\}$

n) The Jacobi identity states that for Poisson brackets featuring three functions on phase space A, B and C the following identity holds:

$$\{\{A, B\}, C\} + \{\{C, A\}, B\} + \{\{B, C\}, A\} = 0.$$

Suppose that A, B and C do not explicitly depend on t. Use (without proof) the Jacobi identity to show that if A and B are two functions on phase space that are conserved then their Poisson bracket is also conserved. (Whilst this can be a useful tool for generating new conserved quantities, it can also generate trivial ones, such as zero or another constant, or merely reproduce A or B or functions of them.)

3) Fourier series as a change of basis: Imagine the set of all square-integrable complex-valued functions, $\phi(x)$, on the interval $0 \le x \le 2\pi$. According to Fourier, such functions may be represented as a superposition of plane waves,

$$\phi(x) = \sum_{n=-\infty}^{\infty} \phi_n \, \frac{1}{\sqrt{2\pi}} \, \mathrm{e}^{inx},$$

where the complex Fourier coefficients $\{\phi_n\}_{n=-\infty}^{\infty}$ are determined from

$$\phi_n = \int_0^{2\pi} dx \, \phi(x) \, \frac{1}{\sqrt{2\pi}} \, \mathrm{e}^{-inx}.$$

a) Compute the quantity ϕ_n for the case that $\phi(x) = x$.

b) Compute $\int_0^{2\pi} dx \, |\phi(x)|^2$ in terms of $\{\phi_n\}_{n=-\infty}^{\infty}$.

c) Regard $\phi(x)$ as the x-component of the vector $\mathbf{F}$ along the basis vector $\mathbf{V}_x$; then

$$\mathbf{F} = \int_0^{2\pi} dx \, \phi(x) \, \mathbf{V}_x.$$

Suppose we change basis from $\{\mathbf{V}_x\}$ to $\{\tilde{\mathbf{V}}_n\}$, where

$$\mathbf{V}_x = \sum_{n=-\infty}^{\infty} \tilde{\mathbf{V}}_n \, \frac{1}{\sqrt{2\pi}} \, \mathrm{e}^{-inx}.$$

Show that, in terms of the new basis, $\{\tilde{\mathbf{V}}_n\}$, the vector $\mathbf{F}$ is given by

$$\mathbf{F} = \sum_{n=-\infty}^{\infty} \phi_n \, \tilde{\mathbf{V}}_n \, .$$

d) Given that the new basis $\{\tilde{\mathbf{V}}_n\}$ is orthonormal, *i.e.*, $\tilde{\mathbf{V}}_n \cdot \tilde{\mathbf{V}}_m = \delta_{nm}$, compute the inner product of $\mathbf{F}$ with itself, in terms of a summation over n.

e) Evaluate the inner products between the original basis vectors, *i.e.*, $\mathbf{V}_x \cdot \mathbf{V}_y$.

f) Evaluate the inner product $\tilde{\mathbf{V}}_n \cdot \mathbf{V}_x$.

g) Compute the inner product of $\mathbf{F}$ with itself by using the representation in terms of the basis $\{\mathbf{V}_x\}$.

h) Show that $\phi(x) = \mathbf{V}_x \cdot \mathbf{F}$ and $\phi_n = \tilde{\mathbf{V}}_n \cdot \mathbf{F}$.

i) Now use Dirac notation rather than bold-face notation for vectors. Then

$$\begin{aligned}
\mathbf{V}_x &\to |x\rangle, \\
\tilde{\mathbf{V}}_n &\to |n\rangle, \\
\mathbf{F} &\to |F\rangle, \\
\mathbf{T} \cdot \mathbf{U} &\to \langle T|U\rangle, \text{ and} \\
|F\rangle &= \int_0^{2\pi} dx \, \phi(x) \, |x\rangle = \sum_{n=-\infty}^{\infty} \phi_n \, |n\rangle \, .
\end{aligned}$$

Show that

$$|F\rangle = \int_0^{2\pi} dx \, |x\rangle \, \langle x|F\rangle = \sum_{n=-\infty}^{\infty} |n\rangle \, \langle n|F\rangle \, .$$

4) Energy conservation – optional: Consider a system of N interacting particles moving in one dimension.

a) Show that if the lagrangean $\mathcal{L}$ has no explicit time dependence, *i.e.*, if $\partial\mathcal{L}/\partial t = 0$, then the quantity $\Gamma \equiv \sum_{i=1}^{N} (\dot{q}^i \, \partial\mathcal{L}/\partial\dot{q}) - \mathcal{L}$ is conserved.

b) Give a physical interpretation of the quantity Γ.

c) Suppose $\mathcal{L}$ is given by $T - V$, where the kinetic energy T and the potential energy V are given by

$$\begin{aligned} T &= \sum_{i=1}^{N} \frac{m}{2} (\dot{q}^i)^2, \\ V &= \sum_{1 \le i < j \le N} U(q^i - q^j) + \sum_{1 \le i \le N} W(q^i). \end{aligned}$$

c.i) Construct Γ in terms of q^i and $\dot{q}^i$; and

c.ii) Construct Γ in terms of T and V.