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PHY422/820: Classical Mechanics

FS 2020

Worksheet #13 (Nov 23 – Nov 25)

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1 Preparation

- Lemos, Chapter 7 (skip 7.4, 7.6-7.7 optional)
- Goldstein, Chapter 8 (skip 8.4, 8.3 optional)

2 Hamiltonian Mechanics

In the next couple of weeks, we will discuss the **Hamiltonian formulation** of Classical Mechanics. We will see that it does not really add new capabilities — in fact, it usually relies on prior knowledge of the Lagrangian and the generalized coordinates — but it brings new insights into the mathematical and geometrical structures of Classical Mechanics. The generalization of these structures were key in the development of both Statistical and Quantum Mechanics.

2.1 Phase Space and the Definition of the Hamiltonian

The setting of Hamiltonian mechanics is the **phase space** of configurations

$$(q_1(t), \ldots, q_n(t), p_1(t), \ldots, p_n(t)) \tag{1}$$

whose evolution will be governed by $2n$ first-order ODEs, instead of the n second-order ODEs for the generalized coordinates q_i in Lagrangian Mechanics. Importantly, the q_i and the **canonical momenta** p_i are treated as **independent variables** in a symmetric fashion. Previously, we saw that

$$p_i(q, \dot{q}, t) = \frac{\partial L}{\partial \dot{q}_i}\,, \tag{2}$$

and we could try to make a change of variables by using these equations to eliminate the $\dot{q}_i$. However, such a naive approach would be non-unique, and therefore non-invertible — clearly, this is not allowed if the Lagrangian and Hamiltonian formulations of mechanics are supposed to be equivalent. To overcome this issue, we change variables by performing a **Legendre transformation** of the Lagrangian (see problem G31). This defines the **Hamiltonian** of a mechanical system:

$$H(q, p, t) = \sum_k p_k \dot{q}_k(q, p, t) - \overline{L}(q, p, t)\,. \tag{3}$$

This matches our definition of the Jacobi integral, but note that the choice of variables is *crucial*: the Jacobi integral is defined on the configuration manifold, not on phase space.

Starting from a Hamiltonian, we can switch to the Lagrangian formalism via the Legendre transformation

$$L(q,\dot{q},t) = \sum_k p_k(q,\dot{q},t)\dot{q}_k - \overline{H}(q,\dot{q},t)\,, \tag{4}$$

where

$$\dot{q}_i(q,p,t) = \frac{\partial H}{\partial p_i}\,. \tag{5}$$

2.2 Hamilton's Equations

In order to derive the governing equations for Hamiltonian dynamics, we consider the total differential of $H(q,p,t)$. Since it is a function of the q_i, p_i and (potentially) t, the differential must have the form

$$dH = \sum_i \left(\frac{\partial H}{\partial q_i}dq_i + \frac{\partial H}{\partial p_i}dp_i\right) + \frac{\partial H}{\partial t}dt\,. \tag{6}$$

The definition via the Legendre transformation of the Lagrangian yields

$$\begin{aligned}
dH &= \sum_i (\dot{q}_i dp_i + p_i d\dot{q}_i) - \sum_i \left(\frac{\partial L}{\partial q_i}dq_i + \frac{\partial L}{\partial \dot{q}_i}d\dot{q}_i\right) - \frac{\partial L}{\partial t}dt \\
&= \sum_i (\dot{q}_i dp_i + p_i d\dot{q}_i) - \sum_i \left(\left(\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i}\right)dq_i + \frac{\partial L}{\partial \dot{q}_i}d\dot{q}_i\right) - \frac{\partial L}{\partial t}dt \\
&= \sum_i (\dot{q}_i dp_i + p_i d\dot{q}_i) - \sum_i (\dot{p}_i dq_i + p_i d\dot{q}_i) - \frac{\partial L}{\partial t}dt \\
&= \sum_i (\dot{q}_i dp_i - \dot{p}_i dq_i) - \frac{\partial L}{\partial t}dt\,.
\end{aligned} \tag{7}$$

Comparing Eqs. (6) and (7), we obtain **Hamilton's equations**

$$\dot{q}_i = \frac{\partial H}{\partial p_i}\,, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}\,, \tag{8}$$

as well as

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}\,. \tag{9}$$

From the latter equation, we see that H is conserved if it does not explicitly depend on time.

Box 2.1: Recipe for Solving Problems in Hamiltonian Mechanics

The general procedure for solving problems in Hamiltonian Mechanics consists of the following steps:

1. Choose generalized coordinates and construct $L(q, \dot{q}, t)$.
2. Construct the canonical momenta p_i, and solve for $\dot{q}_i(q, p, t)$.
3. Perform a Legendre transformation to construct $H(q, p, t)$.
4. Write down Hamilton's equations and solve them.

2.3 Examples

Let us now discuss some examples.

2.3.1 The Harmonic Oscillator

We start from the Lagrangian

$$L = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 \,. \tag{10}$$

The canconical momentum is

$$p = \frac{\partial L}{\partial \dot{q}} = m\dot{q} \,, \quad \dot{q} = \frac{p}{m} \,. \tag{11}$$

Carrying out the Legendre transformation, we obtain the Hamiltonian

$$H = \frac{\partial L}{\partial \dot{q}}\dot{q} - L = \frac{p^2}{m} - \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 \,. \tag{12}$$

Hamilton's equations read

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m} \,, \tag{13}$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -m\omega^2 q \,. \tag{14}$$

The first equation simply reproduces what we found from the introduction of the canonical momentum above, and serves as a consistency check. To solve the coupled ODEs (13)–(13) analytically, we plug one of the equations into the other. In this way, we obtain either

$$\ddot{q} + \omega^2 q = 0 \,, \tag{15}$$

which is solved by the usual ansatz

$$q(t) = q_0 \cos(\omega t + \phi_0) \,, \tag{16}$$

or

$$\ddot{p} + \omega^2 p = 0 \,, \tag{17}$$

with

$$p(t) = p_0 \cos(\omega t + \phi_0) \,. \tag{18}$$

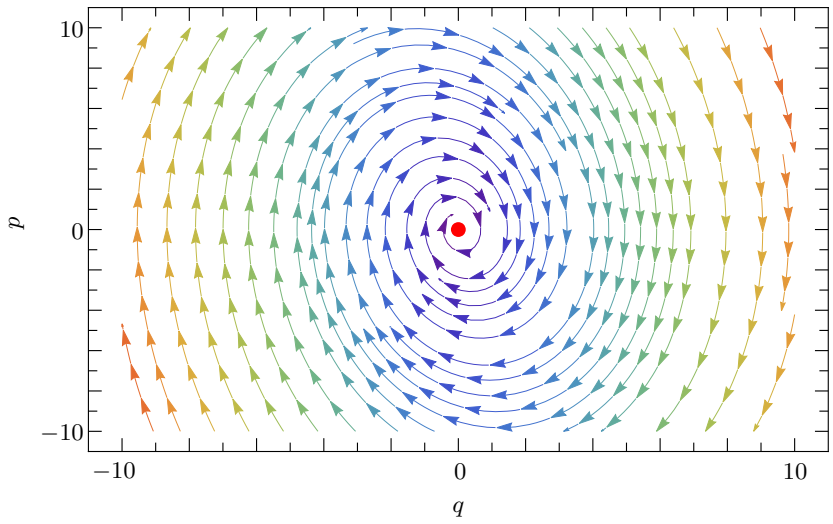

Figure 1: Phase space of an underdamped harmonic oscillator with $\omega_0 = 2\,\mathrm{s}^{-1}$ and $\beta = 1\,\mathrm{s}^{-1}$. The fixed point at the origin is indicated in red.

To obtain the trajectory for the generalized coordinate, we can integrate Eq. (13) to obtain

$$q(t) = -\frac{p_0}{m\omega}\sin(\omega t + \phi_0)\,. \tag{19}$$

Since $\frac{\partial H}{\partial t} = 0$, we also know that H is conserved. In the present example, it corresponds to the total energy, and we can write

$$1 = \frac{H}{E} = \frac{p^2}{2mE} + \frac{q^2}{\frac{2E}{m\omega^2}}\,. \tag{20}$$

This is the definition of an ellipse with semi-axes $a = \sqrt{2mE}$ and $b = \sqrt{2E/m\omega^2}$ in phase space.

Phase Space of the Damped and Driven Harmonic Oscillator

Let us take this opportunity to discuss typical phase space trajectories of a general damped and driven harmonic oscillator, which is described by the equations

$$\dot{q} = \frac{p}{m}\,, \tag{21}$$

$$\dot{p} = -m\omega^2 q - \frac{\beta}{m}p + f_{\mathrm{ext}}\cos\omega_{\mathrm{ext}}t\,. \tag{22}$$

They define the **phase space flow** of the model, a two-dimensional vector field that is tangential to the phase space trajectory at each point (q, p). In Fig. 1 we show this flow for an underdamped oscillator without driving ($f_{\mathrm{ext}} = 0$). We see that regardless of the starting point in phase space, the trajectories will always evolve towards the origin. The origin is an **(attractive) fixed point** of the oscillator's dynamics, which is reached in the limit $t \gg 1$ as the oscillator comes to a rest.

Figure 2 shows the corresponding flow for the overdamped case, in which the oscillator is not able to perform a complete oscillation. As a consequence, the "vorticity" we find in the underdamped case is absent, although the trajectories exhibit some curvature.

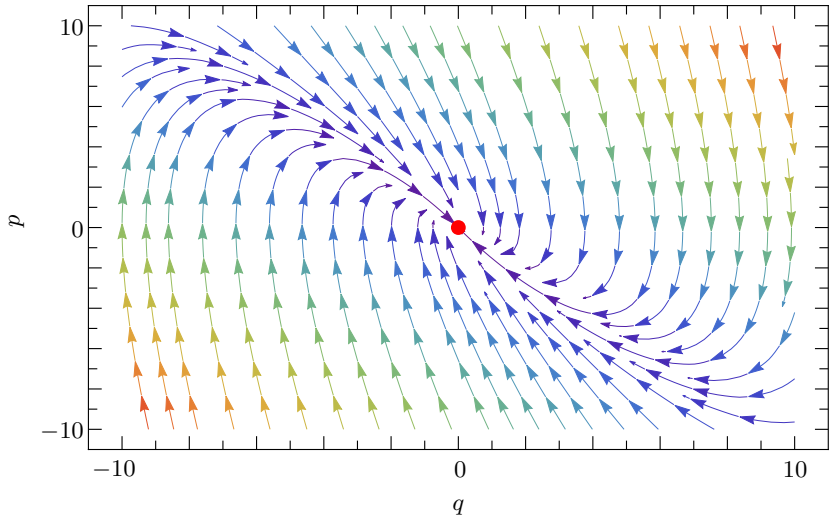

Figure 2: Phase space of an overdamped harmonic oscillator with $\omega_0 = 2\,\mathrm{s}^{-1}$ and $\beta = 1\,\mathrm{s}^{-1}$. The fixed point at the origin is indicated in red.

2.3.2 The Pendulum

[...] Choosing a downward pointing vertical axis, the Lagrangian of the simple pendulum is given by

$$L = T - V = \frac{1}{2}ml^2\dot{\phi}^2 + mgl\cos\phi\,. \tag{23}$$

Introducing the canonical momentum

$$p = \frac{\partial L}{\partial \dot{\phi}} = ml^2\dot{\phi}\,, \tag{24}$$

the Hamiltonian becomes

$$H = \frac{p^2}{2ml^2} - mgl\cos\phi\,. \tag{25}$$

and we can immediately obtain Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p} = \frac{p}{ml^2}\,, \tag{26}$$

$$\dot{p} = -\frac{\partial H}{\partial \phi} = -mgl\sin\phi\,. \tag{27}$$

In Figure 3, we show both the phase space flow as well as several phase space trajectories with constant energy E. We see that for small angles ϕ (or canonical momental p), the trajectories are nearly elliptical, like those of a harmonic oscillator. This is expected in the small-angle limit, as we have seen numerous times.

For larger angles ϕ, the trajectories become increasingly deformed. The intersection points of the trajectories with the $p = 0$ axis at odd multiples of π (i.e., $\phi = (2k+1)\pi, k \in \mathbb{Z}$) are saddle points of the flow. At these points, the pendulum's bob is upside down and at rest, which is obviously an unstable configuration. The phase space curve passing through these points is called the **separatrix** of the pendulum. It is the boundary of the phase space volume that contains the *oscillatory* trajectories of the pendulum from trajectories that are purely *rotational*. In Fig. 3, these rotational trajectories are periodic in p but unbounded in ϕ in the sense that we allow multiple revolutions by allowing $\phi \in]-\infty, \infty[$. [...]

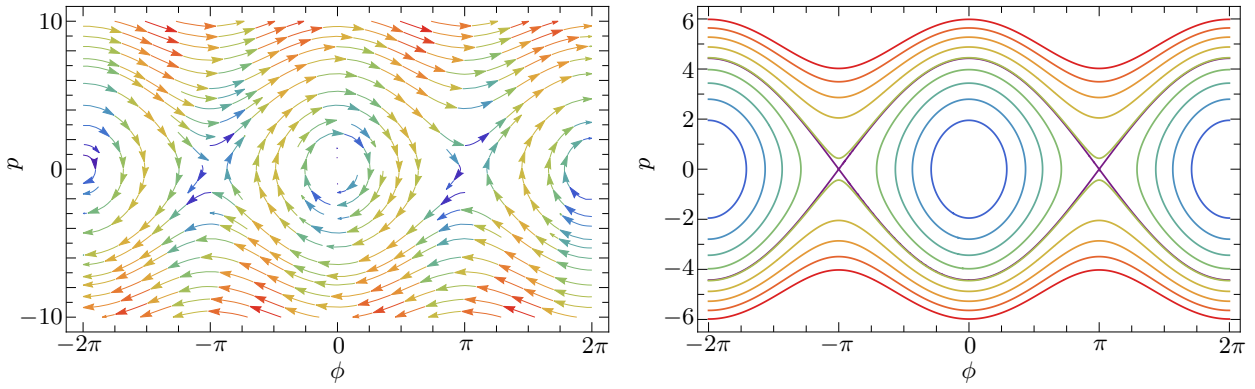

Figure 3: *Left:* Phase space flow of the simple pendulum. *Right:* Isoenergetic phase space trajectories.

2.3.3 The Van der Pol Oscillator

[...]

The Van der Pol oscillator is described by the equations

$$\dot{q} = \frac{p}{ml^2}\,, \tag{28}$$

$$\dot{p} = -m\omega^2 q + \mu(1-q^2)p\,. \tag{29}$$

Its phase space flow for $\mu = 1$ and $\omega_0 = 2\mathrm{s}^{-1}$ is shown in Fig. 4: At large times, any trajectory of the oscillator will be attracted to the **limit cycle** that is shown in the figure in red.

[...]

2.4 Hamilton's Equations from a Variational Principle

3 The Virial Theorem

3.1 Statement and Proof

The mean value of a time-dependent function $f(t)$ can be defined as

$$\left\langle\, f \,\right\rangle = \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau dt\, f(t)\,. \tag{30}$$

For an integrable periodic function with period T, the limit is guaranteed to exist and we have

$$\left\langle\, f \,\right\rangle = \frac{1}{T} \int_0^T dt\, f(t)\,. \tag{31}$$

Let us now consider a dynamical system with canonical coordinates (q, p) that is governed by the Hamiltonian $H(q, p, t)$. We can introduce the so-called **(generalized) virial**

$$\mathcal{V} \equiv -\sum_i q_i \frac{\partial H}{\partial q_i}\,, \tag{32}$$

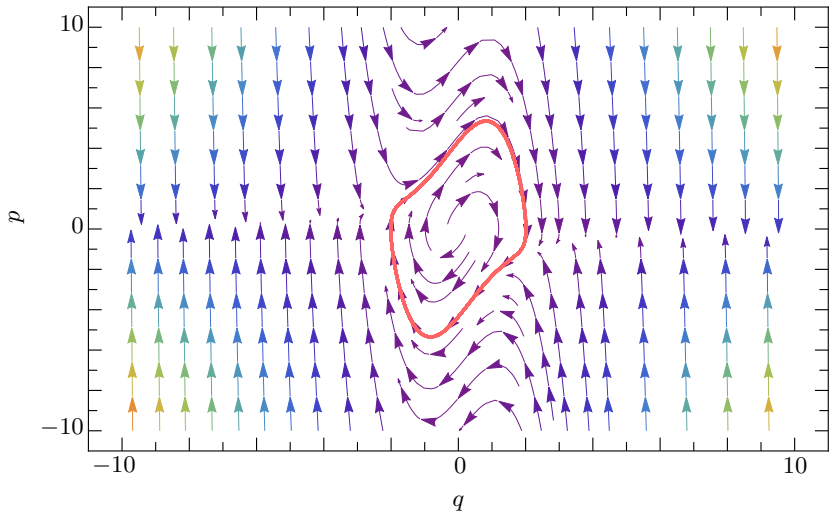

Figure 4: Phase space of the Van der Pol oscillator with $\mu = 1$ and $\omega_0 = 2\text{s}^{-1}$. The limit cycle is indicated in red.

Virial Theorem

If $q_i(t)$ and $p_i(t)$ are bounded functions and if the mean values of the quantities $\sum_i q_i \frac{\partial H}{\partial q_i}$ and $\sum_i p_i \frac{\partial H}{\partial p_i}$ exist separately, then they are equal:

$$\left\langle \sum_i q_i \frac{\partial H}{\partial q_i} \right\rangle = \left\langle \sum_i p_i \frac{\partial H}{\partial p_i} \right\rangle . \tag{33}$$

which can be related to the mean value of other dynamical quantities under certain circumstances.

In order to prove this theorem, we introduce a function

$$G(t) \equiv \sum_i p_i(t) q_i(t) . \tag{34}$$

Since we demanded that the q_i and p_i are bounded, $G(t)$ will be bounded as well. Differentiating G with respect to time and using Hamilton's equations, we have

$$\dot{G} = \sum_i (p_i \dot{q}_i + \dot{p}_i q_i) = \sum_i \left(p_i \frac{\partial H}{\partial p_i} - q_i \frac{\partial H}{\partial q_i} \right) . \tag{35}$$

Taking the mean value on both sides, we obtain

$$\left\langle \dot{G} \right\rangle = \left\langle \sum_i \left(p_i \frac{\partial H}{\partial p_i} - q_i \frac{\partial H}{\partial q_i} \right) \right\rangle . \tag{36}$$

We also have

$$\left\langle \dot{G} \right\rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt \, \frac{dG}{dt} = \lim_{\tau \to \infty} \frac{G(\tau) - G(0)}{\tau} = 0 , \tag{37}$$

because $\tau \to \infty$ while the terms in the numerator were bounded by construction. Provided both of the mean values on the right-hand side exist separately, we see that

$$\langle\, \dot{G} \,\rangle = \Big\langle \sum_i \left(p_i \frac{\partial H}{\partial p_i} - q_i \frac{\partial H}{\partial q_i} \right) \Big\rangle = \Big\langle \sum_i p_i \frac{\partial H}{\partial p_i} \Big\rangle - \Big\langle \sum_i q_i \frac{\partial H}{\partial q_i} \Big\rangle = 0\,, \tag{38}$$

which completes our proof.

3.2 Applications

3.2.1 Central-Force Motion

Let us apply the virial theorem to the motion of an object under a central force, whose Hamiltonian is given by

$$H = \frac{\vec{p}^{\,2}}{2m} + V(r)\,. \tag{39}$$

Evaluating the mean values in Cartesian coordinates for simplicity, we have

$$\Big\langle \sum_i p_i \frac{\partial H}{\partial p_i} \Big\rangle = \Big\langle \frac{\vec{p}^{\,2}}{m} \Big\rangle = 2\,\langle\, T \,\rangle \tag{40}$$

and

$$\Big\langle \sum_i r_i \frac{\partial H}{\partial r_i} \Big\rangle = \Big\langle\, \vec{r} \cdot \vec{\nabla} V(r) \,\Big\rangle = \Big\langle\, \vec{r} \cdot \frac{dV}{dr} \frac{\vec{r}}{r} \Big\rangle = \Big\langle\, r \frac{dV}{dr} \,\Big\rangle\,. \tag{41}$$

For a power-law potential,

$$V(r) = A r^n \tag{42}$$

the virial theorem therefore implies that

$$2\,\langle\, T \,\rangle = n\,\langle\, V \,\rangle\,, \tag{43}$$

and the mean energy must satisfy

$$E = \langle\, E \,\rangle = \langle\, T \,\rangle + \langle\, V \,\rangle = \frac{n+2}{n}\,\langle\, T \,\rangle = \left(1 + \frac{n}{2}\right) \langle\, V \,\rangle \tag{44}$$

For a Kepler-Coulomb type potential ($n = 1$), we specifically have

$$E = -\,\langle\, T \,\rangle = -\frac{1}{2}\,\langle\, V \,\rangle\,, \tag{45}$$

which shows that bound orbits have a negative energy. For the isotropic oscillator ($n = 2$), we obtain

$$\langle\, T \,\rangle = \langle\, V \,\rangle\,. \tag{46}$$

3.2.2 Equation of State of an Ideal Gas

The virial theorem can be used to derive the equation of state of an ideal gas in an efficient manner. Such a gas consists of a large number of non-interacing particles that would be described by the free Hamiltonian

$$H_{\text{free}} = \sum_i \frac{\vec{p}_i^{\,2}}{2m}\,. \tag{47}$$

Let us assume that the gas is contained in a closed volume V, whose walls provide a confining potential $U(\vec{r}_i)$ for each particle:

$$H_{\text{free}} = \sum_i \left(\frac{\vec{p}_i^{\,2}}{2m} + U(\vec{r}_i) \right) . \tag{48}$$

The virial theorem now implies that

$$2 \left\langle T \right\rangle = \left\langle \sum_i \vec{r}_i \cdot \vec{\nabla}_i U \right\rangle = - \left\langle \sum_i \vec{r}_i \cdot \vec{F}_i \right\rangle . \tag{49}$$

The force $\vec{F}_i$ the gas molecules experience is solely due to the collision with the wall, which allows us to relate the *mean force* experienced by the gas to the *pressure* on the walls of the volume. For a small area element of the wall, we have

$$d\vec{F} = -P d\vec{A} = -P \vec{n} dA \,, \tag{50}$$

where $\vec{n}$ is the unit vector of the surface. Thus, we can write

$$- \left\langle \sum_i \vec{r}_i \cdot \vec{F}_i \right\rangle = - \oint_{\partial V} \vec{r} \cdot d\vec{F} = P \oint_{\partial V} \vec{r} \cdot d\vec{A} , \tag{51}$$

where we have used that the pressure is constant. Using Gauss' Law, we see that

$$\oint_{\partial V} \vec{r} \cdot d\vec{A} = \int_V \vec{\nabla} \cdot \vec{r} \, dV = 3 \int_V dV = 3V \,, \tag{52}$$

Recalling the *equipartition theorem*, we can write the average kinetic energy of the gas as

$$\left\langle T \right\rangle = N \cdot \frac{3}{2} k_B \mathcal{T} \,, \tag{53}$$

where N is the number of gas molecules, k_B is the Boltzmann constant, and $\mathcal{T}$ is the absolute temperature. Combining our results, Eq. (49) yields

$$2 \left\langle T \right\rangle = 3 N k_B \mathcal{T} = 3PV \,, \tag{54}$$

and we obtain the equation of state of the ideal gas:

$$PV = N k_B \mathcal{T} \,. \tag{55}$$

4 Group Exercises

Problem G31 – Legendre Transformations

Consider the following situation: We know a function $f(x, y)$ that relates two quantities x and y, but we would rather have a relationship $\tilde{f}(x, z)$ where $z = \frac{\partial f}{\partial y}$ is of greater interest to us, e.g., because it can be measured more readily, or because it might be conserved (an example would be $L(q, \dot{q})$, with $p = \frac{\partial L}{\partial \dot{q}}$ being a conserved momentum).

1. **The naive approach:** Consider the family of functions

$$f_a(x, y) = x^2 + (y - a)^2 \,. \tag{56}$$

   Determine $\tilde{f}_a(x, z) = f_a(x, y(x, z))$ by computing $z = \frac{\partial f_a}{\partial y}$, solving the resulting equation for y, and plugging this $y(x, z)$ into the original function. Show that the relationship between f_a and $\tilde{f}_a$ is not unique, which means that we cannot invert the procedure to obtain f_a from $\tilde{f}_a$.

2. **The Legendre transformation:** Compute $z = \frac{\partial f_a}{\partial y}$ as before, and use it to construct the Legendre transform

$$g_a(x, z) \equiv zy(x, z) - f_a(x, y(x, z)) \,. \tag{57}$$

   Show that the transformation is invertible, i.e., that we can compute $y = \frac{\partial g_a}{\partial z}$ and obtain the original function from

$$f_a(x, y) = yz(x, y) - g_a(x, z(x, y)) \,. \tag{58}$$

   How are $\frac{\partial g_a}{\partial x}$ and $\frac{\partial f_a}{\partial x}$ related?

Problem G32 – An Abstract Hamiltonian

[**adapted from Goldstein 8.14**] The Lagrangian for a system can be written as

$$L = a\dot{x}^2 + b\frac{\dot{y}}{x} + c\dot{x}\dot{y} + fy^2\dot{x}\dot{z} + g\dot{y} - k\sqrt{x^2 + y^2} \,. \tag{59}$$

1. Construct the Hamiltonian.

2. Use Hamilton's equations to identify conserved quantities.