1. Basics of Classical Mechanics

Earlier we have considered stochastic differential equations describing laws of motion of particles, such as the Langevin dynamics and the over damped Langevin dynamics. How we are going to explore where these SDEs come from. We start with some basics of classical mechanics.

1.1. Action functional, Lagrangian, and the Euler-Lagrange Equation. Consider $N$ particles moving in $\mathbb{R}^d$. Set $n := Nd$. Let $\mathbf{q} \in \mathbb{R}^n$ be the vector describing the positions of the particles. Then the vector

$$\dot{\mathbf{q}} := \frac{d\mathbf{q}}{dt}$$

is the vector of velocities of the particles. We postulate that the particles obey the Minimal Action Principle. This means that they move from the position vector $\mathbf{q}_0 := \mathbf{q}(t_0)$ to the position vector $\mathbf{q}_1 := \mathbf{q}(t_1)$ in such a way that the action functional

$$A(\mathbf{q}) := \int_{t_0}^{t_1} \mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t) dt$$

is minimal possible. The function $\mathcal{L}(\mathbf{q}, \dot{\mathbf{q}}, t)$ in the action functional is called the Lagrangian. The necessary condition for a path $\mathbf{q}(t)$ to be a minimizer of the action (1) is that it must be its extremal. Let $\mathbf{q}(t)$ be a path minimizing the action (1) and satisfying the boundary conditions $\mathbf{q}(t_0) = \mathbf{q}_0$ and $\mathbf{q}(t_1) = \mathbf{q}_1$. Suppose we perturb the path $\mathbf{q}(t)$ so that it
still satisfies the boundary conditions, i.e., we consider another path $q(t) + \delta q(t)$ where $\delta q(t_0) = \delta q(t_1) = 0$. Since $A(q, \dot{q})$ achieves its minimum on $q$, we should have

$$A(q + \delta q) \geq A(q).$$

Consider the variation of the action $A$, i.e., the difference between $A(q + \delta q)$ and $A(q + \delta q)$:

$$\delta A := A(q + \delta q) - A(q) = \int_{t_0}^{t_1} [L(q + \delta q, \dot{q} + \delta \dot{q}, t) - L(q, \dot{q}, t)] \, dt.$$

We want to obtain conditions on the path $q(t)$ under which $\delta A = O(\delta q^2, \delta \dot{q}^2)$, i.e., the variation $\delta A$ has no linear terms with respect to $\delta q$ and $\delta \dot{q}$. Otherwise, the path $q(t)$ will not minimize the action.

To calculate the variation $\delta A$, we write a Taylor expansion of $L(q + \delta q, \dot{q} + \delta \dot{q})$ around $L(q, \dot{q})$:

$$L(q + \delta q, \dot{q} + \delta \dot{q}, t) = L(q, \dot{q}, t) + \sum_{i=1}^{n} \delta q_i \frac{\partial L}{\partial q_i} + \sum_{i=1}^{n} \delta \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} + O(\delta q^2, \delta \dot{q}^2)$$

$$\equiv L(q, \dot{q}, t) + \delta q \cdot \nabla_q L + \delta \dot{q} \cdot \nabla_{\dot{q}} L + O(\delta q^2, \delta \dot{q}^2).$$

Plugging the expansion (3) into Eq. (2) and integrating the term $\delta \dot{q} \cdot \nabla_{\dot{q}} L$ by parts taking into account that $\delta q(t_0) = \delta q(t_1) = 0$, we obtain

$$\delta A = \int_{t_0}^{t_1} [\delta q \cdot \nabla_q L + \delta \dot{q} \cdot \nabla_{\dot{q}} L + O(\delta q^2, \delta \dot{q}^2)] \, dt$$

$$= \int_{t_0}^{t_1} \left[ \delta q \cdot \left( \nabla_q L - \frac{d}{dt} \nabla_{\dot{q}} L \right) + O(\delta q^2, \delta \dot{q}^2) \right] \, dt.$$

In order to kill the linear in $\delta q$ part of the variation $\delta A$ we require that

$$\nabla_q L - \frac{d}{dt} \nabla_{\dot{q}} L = 0.$$

Equation (5) are Lagrange’s equation. If the integrand function in the action (1) is arbitrary, Eq. (5) is called the Euler-Lagrange equation for the functional (1). Written in the coordinate form they become:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0, \quad i = 1, 2, \ldots, n.$$

**Example 1** For Newton’s mechanics, where a body is moving in the potential force field $-\nabla U(q)$, the Lagrangian is the difference between the kinetic and the potential energy:

$$L(q, \dot{q}) = \frac{m|\dot{q}|^2}{2} - U(q).$$
We have omitted the argument \( t \) because \( \mathcal{L} \) does not depend on \( t \) explicitly. The Euler-Lagrange equation is

\[
\nabla_q \mathcal{L} - \frac{d}{dt} \nabla_q \dot{\mathcal{L}} = -\nabla(q) - m \frac{d}{dt} \dot{q} = -\nabla(q) - m \ddot{q} = 0.
\]

Therefore, the Euler-Lagrange equation (8) is the second Newton’s law:

\[
m \ddot{q} = -\nabla U(q).
\]

**Example 2** Consider planar motion in a central force field in polar coordinates. In this case, \( q \equiv r = (r, \phi) \). Central force field means that the force is of the form \( \mathbf{F} = -U'(r) \). In the polar coordinates,

\[
\dot{\mathbf{r}} = \dot{r} \hat{e}_r + r \dot{\phi} \hat{e}_\phi,
\]

where \( \hat{e}_r \) and \( \hat{e}_\phi \) are unit vectors in threnodial direction and in the direction orthogonal to it respectively (see Fig. 1(a)). Therefore, the kinetic energy is given by

\[
T = \frac{m|\dot{\mathbf{r}}|^2}{2} = \frac{m}{2}(\dot{r}^2 + r^2 \dot{\phi}^2).
\]

The Lagrangian is the difference between the kinetic and potential energy:

\[
\mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) = \frac{m}{2}(\dot{r}^2 + r^2 \dot{\phi}^2) - U(r).
\]

The Euler-Lagrange equations are:

\[
\begin{align*}
mr^2 \ddot{\phi} - U'(r) - m \ddot{r} &= 0, \\
m \frac{d}{dt}(r^2 \dot{\phi}) &= 2r \dot{r} \dot{\phi} + r^2 \dddot{\phi} = 0.
\end{align*}
\]

Eq. (11) implies that the quantity \( r^2 \dot{\phi} \) is constant of time. This quantity \( r^2 \dot{\phi} \) has a geometric meaning: it is the sectoral velocity. Its conservation was discovered by Kepler through the observation of the motion of the planets: *in equal times the radius vector sweeps equal areas, so that the sectoral velocity is constant* (see Fig. 1(b)). Sectoral velocity conservation implies conservation of the angular momentum \( M = \mathbf{r} \times \dot{\mathbf{r}} \), where \( \times \) denotes the vector product. Indeed,

\[
M = \mathbf{r} \times \dot{\mathbf{r}} = (r \dot{\mathbf{e}}_r) \times (\dot{r} \dot{\mathbf{e}}_r + r \ddot{\mathbf{e}}_\phi) = \dot{r} \dot{\mathbf{e}}_r \times r \ddot{\mathbf{e}}_\phi + r^2 \dot{\mathbf{e}}_r \times \dddot{\mathbf{e}}_\phi = r^2 \dot{\mathbf{e}}_r \times \dot{\mathbf{e}}_\phi = \mathbf{r} \times \dot{\mathbf{r}}.
\]

as \( \dot{\mathbf{e}}_r \times \dot{\mathbf{e}}_\phi = 0 \). Noting that \( \dot{\mathbf{e}}_r \times \dot{\mathbf{e}}_\phi \) is the unit normal to the plane of the motion and recalling that \( r^2 \dot{\phi} \) is constant we conclude that the angular momentum \( M \) is conserved.
Figure 1. (a): $\mathbf{r}$ and $\dot{\mathbf{r}}$ for the planar motion in the central force field in the polar coordinates. (b): An illustration to Kepler’s law stating that the sectoral velocity is constant in the planar motion in the central force field.

1.2. Legendre Transform. Let $y = f(x)$, $x \in \Omega \subset \mathbb{R}^n$, be a smooth strictly convex function. Strict convexity means that

$$f(tx_1 + (1-t)x_2) < tf(x_1) + (1-t)f(x_2) \quad \text{for all } x_1, x_2 \in \Omega, x_1 \neq x_2, t \in (0, 1).$$

Suppose $f(0) = 0$. Consider the function $F(p, x) := p \cdot x - f(x)$. Due to strict convexity of $f(x)$, for each fixed $p$, one can find a unique point $x(p)$ at which the function $F(p, x) = p \cdot x - f(x)$ assumes its maximum. Now we define

$$g(p) := \max_{x \in \Omega} \{p \cdot x - f(x)\} \equiv F(p, x(p)).$$

The function $g(p)$ is called the Legendre transform of the function $f(x)$. The point $x(p)$ is found from the condition

$$\frac{\partial F(p, x)}{\partial x} \equiv p - \frac{df}{dx} = 0, \quad \text{i.e.,} \quad \frac{\partial f}{\partial x}(x(p)) = p.$$

Exercise Show that under the assumptions above, the Legendre transform is involutive, i.e., its square is identity.

1.3. Hamilton’s equations. Now we pick the lagrangian $L(q, \dot{q})$ to be function $f$ and we apply the Legendre transform to it with respect to the variable $\dot{q}$:

$$\mathcal{H}(p, q, t) = p\dot{q} - L(q, \dot{q}, t).$$
The function \( H(p, q) \) is the Hamiltonian. Since the Legendre transform is involutive, the Legendre transform applied to the Hamiltonian is the Lagrangian:

\[
\mathcal{L}(q, \dot{q}, t) = p\dot{q} - H(p, q, t).
\]

The momentum \( p \) is defined from the condition

\[
p = \frac{\partial \mathcal{L}}{\partial \dot{q}}.
\]

The Euler-Lagrange equation implies that

\[
\dot{p} := \frac{d}{dt} p = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial q}.
\]

Now we will show that Lagrange’s equation (5) is equivalent to the system of Hamilton’s equations

\[
(14) \quad \dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}.
\]

Indeed, the total differential of the Hamiltonian \( H \)

\[
dH = \frac{\partial H}{\partial p} dp + \frac{\partial H}{\partial q} dq + \frac{\partial H}{\partial t} dt
\]

must coincide with the total differential of \( p \cdot \dot{q} - \mathcal{L} \) for \( p = \frac{\partial \mathcal{L}}{\partial q} \):

\[
dH = \dot{q} dp - \frac{\partial \mathcal{L}}{\partial q} dq - \frac{\partial \mathcal{L}}{\partial t} dt.
\]

Therefore,

\[
\dot{q} = \frac{\partial H}{\partial p}, \quad \frac{\partial \mathcal{L}}{\partial q} = \frac{\partial H}{\partial q}, \quad \frac{\partial H}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}.
\]

The equation for \( \dot{q} \) is already there. Using \( \dot{p} = \frac{\partial \mathcal{L}}{\partial q} \) we obtain

\[
\dot{p} = \frac{\partial \mathcal{L}}{\partial p} = -\frac{\partial H}{\partial q}.
\]

**Example 3**  For Newton’s mechanics, where a body is moving in the potential force field \(-\nabla U(q)\), the Hamiltonian is the sum of the kinetic and the potential energy:

\[
H(p, q) = \frac{1}{2m} |p|^2 + U(q).
\]

Hamilton’s equations are

\[
(16) \quad \dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial q} = -\nabla U(q).
\]
Now we show that if the Hamiltonian does not explicitly depend on time then it is a constant during the motion. Indeed,

\[
\frac{dH}{dt} = \frac{\partial H}{\partial p} \frac{dp}{dt} + \frac{\partial H}{\partial q} \frac{dq}{dt} + \frac{\partial H}{\partial t}.
\]

Hence,

\[
\frac{dH}{dt} = \frac{\partial H}{\partial t},
\]

which shows that \( \frac{\partial H}{\partial t} = 0 \) implies \( \frac{dH}{dt} = 0 \).

1.4. The Hamilton-Jacobi equation.

**Definition 1.** Let the initial point \( q_0 \) and the initial time \( t_0 \) be fixed, while the final point \( q \) and the final time \( t \) be variable. We define the action function of the final point and the final time as

\[
S(q_0, t_0)(q, t) = \int_\phi L ds,
\]

where \( \phi(s) \) is the extremal (the minimizer of the action (1)) connecting the points \( (q_0, t_0) \) and \( (q, t) \).

In order for this definition to be correct, i.e., the function \( S(q_0, t_0)(q, t) \) to be uniquely defined for every final point \( (q, t) \) in the domain of consideration, we need to require that the externals emanating from \( (q_0, t_0) \) do not intersect elsewhere. Further we will assume that the initial point \( (q_0, t_0) \) is fixed and omit the subscript of \( S \) for brevity: \( S(q, t) \).

Let us show that the differential of the action function for a fixed initial point is given by

\[
dS = pdq - H dt,
\]

where \( p = \frac{\partial L}{\partial \dot{q}} \) and \( H = p \cdot \dot{q} - L \). We lift every extremal from \( (q, t) \)-space to the extended phase space \( \{(p, q, t)\} \), setting \( p = \frac{\partial L}{\partial \dot{q}} \) (see Fig. 2). Then we get an \( n + 1 \)-dimensional manifold in the \( 2n + 1 \)-dimensional phase space consisting of phase trajectories. Mark the initial and the final points \( (q_0, t_0) \) and \( (q, t) \) as well as their counterparts in the phase space \( (p_0, q_0, t_0) \) and \( (p, q, t) \). Perturb the final point by \( (\Delta q, \Delta t) \) and mark the resulting point \( (q + \Delta q, t + \Delta t) \), its counterpart in the phase space \( (p + \Delta p, q + \Delta q, t + \Delta t) \). For every final point of the form \( (q + \theta \Delta q, t + \theta \Delta t) \), \( \theta \in [0, 1] \) find an extremal connecting the initial point \( (q_0, t_0) \) with it. Lift this set of externals into the phase space as shown in Fig. 2. Then the curvilinear triangle in the space \( (q, t) \) consisting of the externals maps onto the curvilinear quadrangle (the shaded surface in Fig. 2) in the phase space. Denote this quadrangle by \( \sigma \). Recall that \( \mathcal{L} = p\dot{q} - H \). Hence the quadrangle \( \sigma \) consists of the phase
Figure 2. An illustration to the proof of Eq. (18).

Trajectories of the form $p \delta q - H dt$. Show that each phase trajectory $\gamma \subset \{(p, q, t)\}$ is an extremal of

$$\int_\gamma (p \delta q - H dt)$$

for which the endpoints remain in the $n$-dimensional subspaces $(t = t_0, q = q_0)$ and $(t = t_1, q = q_1)$. Indeed,

$$\delta \int_\gamma (p \delta q - H dt) = \int_\gamma \left( p \delta \dot{q} + \dot{q} \delta p - \frac{\partial H}{\partial q} \delta q - \frac{\partial H}{\partial p} \delta p \right) dt$$

$$= p \delta q |_{t_1}^{t_0} + \int_\gamma \left( \dot{q} - \frac{\partial H}{\partial p} \right) dp + \left( \dot{p} + \frac{\partial H}{\partial q} \right) dq dt = 0.$$

Since the surface $\sigma$ consists of extremal we have $\int_\sigma d(p \delta q - H dt) = 0$. On the other hand, this surface integral can be replaced with the integral over the boundary of $\sigma$:

$$0 = \int_\sigma d(p \delta q - H dt) = \left[ \int_{\phi_2} + \int_{\beta} - \int_{\phi_1} - \int_{\alpha} \right] (p \delta q - H dt).$$

Note that $\int_\alpha = 0$ as $dq$ and $dt$ are zero on this segment. Further,

$$\left[ \int_{\phi_2} - \int_{\phi_1} \right] (p \delta q - H dt) = S(q + \Delta q, t + \Delta t) - S(q, t).$$

Thus, we have:

$$\int_{\beta} (p \delta q - H dt) = S(q + \Delta q, t + \Delta t) - S(q, t).$$

Letting $\Delta q \to 0$ and $\Delta t \to 0$ we get

$$\int_{\beta} (p \delta q - H dt) = p \Delta q - H \Delta t + o(\Delta t, \Delta q).$$
This proves formula (18).

**Theorem 1.** The action function $S(q, t)$ satisfies the equation

\begin{equation}
\frac{\partial S}{\partial t} + \mathcal{H}\left(\frac{\partial S}{\partial q}, q, t\right) = 0.
\end{equation}

This is a nonlinear first-order partial differential equation called the Hamilton-Jacobi equation.

**Proof.** We note that

\[ dS(q, t) = \frac{\partial S}{\partial q} dq + \frac{\partial S}{\partial t} dt. \]

Eq. (18) implies that

\[ \frac{\partial S}{\partial q} = p \quad \text{and} \quad \frac{\partial S}{\partial t} = -\mathcal{H}. \]

Therefore,

\[ \frac{\partial S}{\partial t} + \mathcal{H}\left(\frac{\partial S}{\partial q}, q, t\right) = 0. \]

The power of the Hamilton-Jacobi equation is that it gives the relationship between the momentum $p$ and the action function $S$. Often in applications the Hamiltonian has some known constant value. If its value is nonzero, we re-define the Hamiltonian and get a stationary Hamilton-Jacobi equation of the form

\[ \mathcal{H}\left(\frac{\partial S}{\partial q}, q, t\right) = 1. \]

If this value is zero, we get a stationary Hamilton-Jacobi equation of the form

\[ \mathcal{H}\left(\frac{\partial S}{\partial q}, q, t\right) = 0. \]

**Example 4** Consider the boundary value problem for the Eikonal equation

\begin{equation}
F(x)|\nabla T(x)| = 1, \quad T(x) = 0, \quad x \in g.
\end{equation}

Here $x \in \mathbb{R}^n$, $n = 2$ or $3$, $g$ is some subset of $\mathbb{R}^n$. This equation arises, e.g., in seismic analysis, where the wave equation, describing propagation of sound waves inside the Earth, is solved approximately using the *heir frequency approximation*. Then the time $T(x)$ at which the point $x$ is reached by the wave front, obeys the Eikonal equation. The function $F(x)$ is the sound speed inside the Earth. In the forward problem, the speed $F(x)$ is known, and one needs to find $T(x)$. Eq. (20) is a Hamilton-Jacobi equation.
for $T(x)$. It is convenient to introduce the slowness function $s(x) = 1/F(x)$ and rewrite the equation as

$$\frac{1}{2} (|\nabla T(x)|^2 - s^2(x)) = 0.$$ 

We define the Hamiltonian

$$\mathcal{H}(p, x) := \frac{|p|^2}{2} - \frac{s^2(x)}{2} = 0.$$ 

The seismic rays, i.e., the characteristics of the Eikonal equation, the curves along which the travel time is minimal, are defined by Hamilton’s equations

$$\frac{dx}{d\sigma} = \frac{\partial \mathcal{H}}{\partial p} = p,$$

$$\frac{dp}{d\sigma} = -\frac{\partial \mathcal{H}}{\partial x} = s(x)\nabla s(x),$$

$$\frac{dT}{d\sigma} = \nabla T(x) \cdot \frac{dx}{d\sigma} = |p|^2.$$ 

$\sigma$ is a parameter along the rays. It is not the time. The ray equations above can be easily integrated numerically. In simplest cases, it can be done analytically.

**Example 5** Consider the SDE

$$dx = b(x)dt + \sqrt{2\beta^{-1}}dw, \quad x \in \mathbb{R}^n.$$ 

We have established that the quasipotential $U(x)$ obeys the Hamilton-Jacobi equation

$$\nabla U(x) \cdot (\nabla U(x) + 2b(x)) = 0.$$ 

Define the momentum $p = \nabla U$. Define the Hamiltonian

$$\mathcal{H}(p, x) = \frac{|p|^2}{2} + p \cdot b(x) = 0.$$ 

Note that this Hamiltonian is not strictly convex. Therefore we cannot use the methodology of the Legendre transform. Nevertheless, we still can write Hamilton’s equations. They will define the characteristics, or the minimum action paths, and give the evolution of the quasipotential along these paths.

$$\frac{dx}{d\sigma} = \frac{\partial \mathcal{H}}{\partial p} = p + b(x),$$

$$\frac{dp}{d\sigma} = -\frac{\partial \mathcal{H}}{\partial x} = \begin{bmatrix} p \cdot \frac{\partial b}{\partial x_1} \\ \vdots \\ p \cdot \frac{\partial b}{\partial x_n} \end{bmatrix},$$

$$\frac{dU}{d\sigma} = \nabla U(x) \cdot \frac{dx}{d\sigma} = p \cdot (p + b(x)) = \frac{|p|^2}{2}.$$
To obtain the equation for $U$, we used

$$p \cdot (p + b(x)) = \frac{|p|^2}{2} + \frac{|p|^2}{2} + p \cdot b(x) = \frac{|p|^2}{2}.$$

Note that the equation $\frac{dx}{dt} = p + b(x)$ giving the velocity vector of the minimum action paths, is consistent with what we have obtained while deriving the Hamilton-Jacobi equation.

2. Statistical mechanics

2.1. Phase flow and Liouville’s theorem.

**Definition 2.** Consider the initial value problem for an autonomous ODE

$$\dot{x} = f(x), \quad x \in \mathbb{R}^d, \quad x(0) = x_0,$$

where the $f$ is continuously differentiable. Then the phase flow associated with this ODE is the one-parameter group of transformations

$$g^t : x(0) \mapsto x(t).$$

*The group elements are given by*

$$g^t(x) = x + f(x)t + O(t^2), \quad t \to 0.$$

Suppose we have a Hamiltonian system with $n$ degrees of freedom where $n$ is large. Such system evolves according to Hamilton’s equations

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}.$$

Assume that the Hamiltonian $H = H(p,q)$, i.e., it does not depend on time explicitly. The phase space for this system, $(q,p)$, is $2n$-dimensional. We denote it by $\Gamma$.

**Definition 3.** The Hamiltonian phase flow is the one-parameter group of transformations of phase space

$$g^t : (p(0), q(0)) \mapsto (p(t), q(t)).$$

where $p(t)$ and $q(t)$ are solutions of Hamilton’s equations

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}.$$

**Exercise** Show that $\{g^t\}$ is a group.

Liouville’s theorem claims that the phase flow preserves volume:

**Theorem 2.** For any region $D \subset \Gamma$

$$\text{Volume of } g^tD = \text{Volume of } D.$$
This can be reformulated as
\[
\det \frac{\partial (p(t), q(t))}{\partial (p(0), q(0))} = 1,
\]
where the determinant is taken of the matrix of partial derivatives of \( (p(t), q(t)) \) with respect to the initial conditions.

**Proof.**

(1) First we will show that the right-hand side of Hamilton’s equations, i.e., the velocity vector \( u \)

\[
 u := \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} \frac{\partial H}{\partial p} \\ -\frac{\partial H}{\partial q} \end{bmatrix}
\]
is divergence-free, i.e., \( \nabla \cdot u = 0 \). Indeed,

\[
\nabla \cdot u = \frac{\partial}{\partial q} \cdot \frac{\partial H}{\partial p} - \frac{\partial}{\partial p} \cdot \frac{\partial H}{\partial q} = \sum_{i=1}^n \frac{\partial^2 H}{\partial q_i \partial p_i} - \frac{\partial^2 H}{\partial q_i \partial p_i} = 0.
\]

(2) Next we show that if we have any ODE \( \dot{x} = f(x) \) where \( f \) is continuously differentiable and divergence-free, i.e., \( \nabla \cdot f = 0 \), then the corresponding phase flow preserves volume. Denote the volume of the image of a region \( D \subset \Gamma \) under the phase flow at time \( t \) by \( v(t) \). For any \( t \), the formula for changing variables in a multiple integral gives

\[
v(t) = \int_D \det \left( \frac{\partial g^t(x)}{\partial x} \right) dx.
\]

Calculate the matrix of derivatives of \( g^t(x) \) with respect to the initial data \( x \) as \( t \to 0 \):

\[
\frac{\partial g^t(x)}{\partial x} = x + f(x) t + O(t^2).
\]

Now we will use the well-known algebraic fact that for any matrix \( A = (a_{ij}) \),

\[
\det(I + At) = 1 + t \text{Tr}(A) + O(t^2),
\]

where \( \text{Tr}(A) \) is the trace of the matrix \( A \), i.e., the sum of its diagonal entries:

\[
\text{Tr}A = \sum_{i=1}^d a_{ii}.
\]

Eq. (22) can be proved by a direct expansion of the determinant: we get 1 and \( n \) in \( t \), the remaining terms involve \( t^2 \), \( t^3 \), etc. Using Eq. (22) we get:

\[
\det \left( \frac{\partial g^t(x)}{\partial x} \right) = 1 + t \text{Tr} \left( \frac{\partial f}{\partial x} \right) + O(t^2).
\]

Now observe that

\[
\text{Tr} \left( \frac{\partial f}{\partial x} \right) = \nabla \cdot f.
\]
Plugging this into Eq. (21) we obtain

\[ v(t) = \int_D \left( 1 + t \nabla \cdot f + O(t^2) \right) dx. \]

Therefore, the rate of change of the phase volume is

\[ \frac{dv}{dt} \bigg|_{t=t_0} = \int_{D(t_0)} \nabla \cdot f dx. \]

Hence, if \( \nabla \cdot f = 0 \), the volume remains constant in time.

(3) Therefore, in the Hamiltonian phase flow phase volume is preserved.

2.2. Liouville’s Equation. Despite the system evolves according to deterministic equations, due to its high dimensionality, it is virtually impossible to know exact initial conditions \((q(0), p(0))\). Instead, they are drawn from some probability density \(W(q, p, 0)\). Furthermore, often we do not need to keep track of every individual trajectory \((q(t), p(t))\), but need to find some macroscopic quantities (observables) such as energy, mean force, etc, which are averages over a large number of trajectories. A collection of phase trajectories is called an *ensemble*.

One way to do so is to derive an equation that gives the time evolution of the probability density \(W(q, p, t)\). Then one can find the observables as the expectations with respect to this pdf. For example, the energy of the ensemble is

\[ E(t) = \mathbb{E}[\mathcal{H}(p, q)] = \int_{\Gamma} \mathcal{H}(p, q) W(q, p, t) dV, \]

where \(dV\) is an element of volume in the phase space \(\Gamma\) (in the Euclidean space \(\mathbb{R}^{2n}\), \(dV = dq dp\)). Similarly, if \(\Phi(q, p)\) is any other function on the phase space, then its macroscopic version is given by

\[ \mathbb{E}[\Phi(p, q, t)] = \int_{\Gamma} \Phi(p, q, t) W(q, p, t) dV. \]

To derive an equation for the time evolution of the pdf \(W(q, p, t)\) (*Liouville’s equation*), consider a volume \(V \subset \Gamma\). The probability for a phase trajectory \((q(t), p(t))\) to be in this volume is

\[ \int_V W(q, p, t) dV. \]

Since the phase trajectories do not appear and do not disappear, the change of this probability comes purely from inflow and outflow of the trajectories through the boundary \(\partial V\) of this volume, i.e.,

\[ \frac{d}{dt} \int_V WdV = - \int_V W u \cdot n dS = - \int_V \nabla \cdot (W u) dV, \]
where \( \mathbf{u} := \begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} \) is the velocity vector of the trajectory, and \( \mathbf{n} \) is the outer unit normal to \( \partial V \). Assuming that the pdf \( W \) is smooth and letting \( V \to 0 \), we deduce that
\[
\frac{\partial W}{\partial t} + \nabla \cdot (W \mathbf{u}) = 0.
\]

Now we will simplify the second term. Note that
\[
\nabla \cdot (W \mathbf{u}) = \nabla W \cdot \mathbf{u} + W \nabla \cdot \mathbf{u}.
\]

In the proof of Liouville’s theorem we have shown that the velocity vector \( \mathbf{u} \) is divergence-free, i.e., \( \nabla \cdot \mathbf{u} = 0 \). Therefore, we obtain \textit{Liouville’s equation}
\[
\frac{\partial W}{\partial t} + \mathbf{u} \cdot \nabla W = 0.
\]

(23)

Liouville’s equation is analogous to the Fokker-Planck equation in the stochastic case. Note that the Liouville equation is first order, while the Fokker-Planck equation is first order in time and second order in phase variables.

Define the Liouville operator as
\[
L := \sum_{i=1}^{n} \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial}{\partial p_i}.
\]

Then the Liouville equation can be rewritten as
\[
\frac{\partial W}{\partial t} = -LW.
\]

(24)

Another form of Liouville’s equation encountered in the literature is
\[
\frac{\partial W}{\partial t} + \{W, \mathcal{H}\} = 0,
\]

(25)

where \( \{f, g\} \) is \textit{the Poisson bracket} defined by
\[
\{f, g\} := \sum_{i=1}^{n} \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i}.
\]

Now we will discuss stationary probability distributions, i.e., such that \( LW = 0 \) which means that \( W \) does not change with time. Show that if \( W(\mathbf{q}, \mathbf{p}) = \Phi(\mathcal{H}(\mathbf{q}, \mathbf{p})) \), i.e., the pdf is a function only of the Hamiltonian, then it is stationary. Indeed,
\[
\mathbf{u} \cdot \nabla \Phi(\mathcal{H}) = \sum_{i=1}^{n} \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \Phi(\mathcal{H})}{\partial q_i} - \frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial \Phi(\mathcal{H})}{\partial p_i}
\]
\[
= \frac{d\Phi}{d\mathcal{H}} \sum_{i=1}^{n} \left[ \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \mathcal{H}}{\partial q_i} - \frac{\partial \mathcal{H}}{\partial q_i} \frac{\partial \mathcal{H}}{\partial p_i} \right] = 0
\]
In particular, the canonical pdf
\[ W(q,p) = \frac{1}{Z} \exp \{-\beta H(q,p)\}, \]
where \( \beta = (k_B T)^{-1} \), is stationary. What is special about it, will be clear from the discussion on entropy.

3. Entropy

3.1. Where the definition of entropy comes from. Consider the problem of distributing \( N \) objects among \( M \) bins, where \( N \gg M \gg 1 \). The number of ways to divide \( N \) objects among \( M \) bins so that each bin \( i \) contains \( n_i \) objects (naturally, \( \sum_{i=1}^{M} n_i = N \)) is
\[ W(n_1, n_2, \ldots, n_M) = \frac{N!}{n_1! n_2! \ldots n_M!}. \]
Let us find out, for which set of numbers \( n_1, \ldots, n_M \) the number of ways \( W(n_1, n_2, \ldots, n_M) \) is maximal. For large \( n \),
\[
\log n! = \log 1 + \log 2 + \ldots + \log n \approx \int_1^n \log x \, dx = x(\log x - 1)|_1^n = n \log n - n + 1 \approx n \log \left( \frac{n}{e} \right) = \log \left( \frac{n}{e} \right)^n.
\]
Therefore,
\[
W \approx \left( \frac{N}{e} \right)^N \frac{n_1^n}{(n_1/e)^{n_1}} \ldots \frac{n_M^n}{(n_M/e)^{n_M}}.
\]
Hence
\[
\log W \approx N \log N - \sum_{i=1}^{M} n_i \log n_i.
\]
Since the logarithm is a monotone function, the configuration maximizing \( W \) also maximizes its logarithm. Define the function
\[
S(n_1, \ldots, n_M) := -\sum_{i=1}^{M} n_i \log n_i.
\]
This function is called (combinatorial) entropy. Maximize it subject to the condition \( n_1 + \ldots + n_M = N \). This can be readily done using the method of Lagrange’s multipliers. Define Lagrange’s function
\[
\Lambda(n_1, \ldots, n_M, \lambda) := -n_1 \log n_1 - \ldots - n_M \log n_M + \lambda(n_1 + \ldots + n_M - N)
\]
and solve the system
\[
\begin{align*}
\frac{\partial \Lambda}{\partial n_i} &= -\log n_i - 1 + \lambda = 0, \quad i = 1, \ldots, M, \\
\frac{\partial \Lambda}{\partial \lambda} &= n_1 + \ldots + n_M - N = 0.
\end{align*}
\]
Solving this system we obtain

\[ n_1 = \ldots = n_m = N/M. \]

Therefore, the entropy is maximized when the distribution of \( N \) objects among \( M \) bins where \( N \gg M \gg 1 \) is uniform. Note that the uncertainty of in which bin a particular object is, is maximized if the objects are distributed uniformly. In this sense, the entropy is a measure of uncertainty.

The quantities \( P_i := n_i/N, \ i = 1, \ldots, M \) are the probabilities to find a given object in \( i \)-th bin. The number of ways \( W \) can be rewritten in terms of \( P_i \)'s:

\[
W \approx \frac{N^N}{n_1^{n_1} \ldots n_M^{n_M}} = \left[ P_1^{P_1} \ldots P_M^{P_M} \right]^{-N}.
\]

Then

\[
\log W = -N \sum_{i=1}^{M} P_i \log P_i.
\]

One can define the probabilistic entropy by

\[
(26) \quad S(P_1, \ldots, P_i) := -\sum_{i=1}^{M} P_i \log P_i.
\]

It differs from the combinatorial entropy by the multiplicative constant \( N \).

Motivated by Eq. (26), one can define entropy associated with a pdf \( f(x), x \in \mathbb{R}^d \):

\[
(27) \quad S = -\int_{\mathbb{R}^d} f(x) \log f(x) dx.
\]

3.2. Entropy and the canonical pdf. Now we will show that the canonical pdf

\[
\mu(\mathcal{H}) = Z^{-1} e^{-\beta \mathcal{H}}, \quad Z = \int_{\Gamma} e^{-\beta \mathcal{H}} dV,
\]

where \( \Gamma \) is the phase space and \( dV = \delta p \delta q \) is the volume element, is the invariant pdf that maximizes the entropy. Suppose we have measured the energy of the ensemble:

\[
E = \mathbb{E}[\mathcal{H}].
\]

We say that a pdf \( W \) is compatible with the measurement if

\[
E = \int_{\Gamma} \mathcal{H} W(\mathcal{H}) dV.
\]

We assume that every pdf that we are considering is compatible with the measurement.

We will show that \( S(m) \geq S(W) \) for any \( W \) comestible with the measurement. The proof is done by the following trick. Consider the function

\[
\psi(x) := \int_{1}^{x} \log t dt = x \log x - x + 1.
\]

Note that

\[
\psi(1) = 0, \ \psi'(x) > 0 \text{ for } x > 1, \text{ and } \psi'(x) < 0 \text{ for } x \in (0, 1).
\]
Therefore,
\[(28) \quad \psi(x) > 0 \text{ for } x \in (0, 1) \cup (1, +\infty).\]

Set \( x = \frac{W}{\mu} \). Since \( m \) and \( W \) are pdf’s and \( \mu > 0 \) everywhere, we have \( x \geq 0 \). Eq. (28) implies that
\[
\frac{W}{\mu} \log \frac{W}{\mu} - \frac{W}{\mu} + 1 = \frac{W}{\mu} (\log W - \log \mu) - \frac{W}{\mu} + 1 \geq 0.
\]

Multiplying by \( \mu \) and regrouping the terms we get
\[
W \log W - W \log \mu \geq W - \mu.
\]

Integrating over the phase space \( \Gamma \) and taking into account that \( \int_{\Gamma} WdV = \int_{\Gamma} \mu dV = 1 \) we obtain:
\[
- \int_{\Gamma} W \log \mu dV \geq - \int_{\Gamma} W \log W dV \equiv S(W).
\]

Note that
\[
\log \mu = - \log Z - \beta \mathcal{H}, \quad \text{and hence} \quad - \int_{\Gamma} W \log \mu dV = \log Z + \beta E,
\]
as \( W \) is compatible with the measurement. On the other hand,
\[
S(\mu) = - \int_{\Gamma} m \log \mu dV = \log Z + \beta E = - \int_{\Gamma} W \log \mu dV.
\]

Therefore,
\[
- \int_{\Gamma} W \log \mu dV = \log Z + \beta E = S(\mu) \geq S(W).
\]

Hence out of all pdf’s compatible with the measurement, the canonical pdf \( \mu(\mathcal{H}) \) maximizes the entropy. While proving this fact, we also have shown that for the canonical pdf \( \mu(\mathcal{H}) \),
\[
(29) \quad S = \log Z + \beta E.
\]

Also note that the parameter \( \beta \) is determined from the equation
\[
E = \mathbb{E}[\mathcal{H}] = \int_{\Gamma} Z^{-1} \mathcal{H} e^{-\beta \mathcal{H}} dV = \frac{\int_{\Gamma} \mathcal{H} e^{-\beta \mathcal{H}} dV}{\int_{\Gamma} e^{-\beta \mathcal{H}} dV} \equiv - \frac{\partial}{\partial \beta} \log \int_{\Gamma} e^{-\beta \mathcal{H}} dV = - \frac{\partial}{\partial \beta} \log Z.
\]

Therefore,
\[
(30) \quad E = - \frac{\partial}{\partial \beta} \log Z.
\]

Note that the normalization constant \( Z \) is temperature-dependent. \( Z \) is also referred to as the partition function.
3.3. **Temperature.** The temperature of the system is defined by the equation

$$T^{-1} = \frac{\partial S}{\partial E}. \tag{31}$$

Eq. (29) implies that if the system is distributed according to the canonical density then

$$T = \beta^{-1}.$$

3.4. **Example: A system of $N$ noninteracting particles.** Consider a system of $N$ noninteracting particles on mass $m$ locked in the volume $V \subset \mathbb{R}^3$. The Hamiltonian is given by

$$\mathcal{H}(p, q) = \sum_{i=1}^{3N} \frac{p_i^2}{2m}.$$ 

The partition function $Z$ is given by

$$Z = \int_{\Gamma} e^{-\beta \mathcal{H}} dpdq = \left( \int_{V} dx dy dz \right)^N \left( \int_{-\infty}^{\infty} e^{-p^2/2m \frac{dp}{d}} \right)^{3N} = V^N \left( \frac{2\pi m}{\beta} \right)^{3N/2}.$$ 

Calculate its logarithm:

$$\log Z = N \log V + \frac{3N}{2} (\log 2\pi m - \log \beta).$$ 

The energy of the system is

$$E = \mathbb{E}[\mathcal{H}] = -\frac{\partial \log Z}{\partial \beta} = \frac{3N}{2} \beta^{-1} = \frac{3N}{2} T.$$ 

Therefore, the energy per degree of freedom is $T/2$. The entropy is given by

$$S = \log Z + \beta E = \log Z + \frac{3N}{2}.$$ 

Recall that the free energy is defined by

$$\mu_{\mathcal{H}}(E) = Z^{-1} \int_{\Gamma} e^{-\beta \mathcal{H}(p, q)} \delta(\mathcal{H}(p, q) - E) dpdq = Z^{-1} e^{-\beta E} \Omega(E),$$

where

$$\Omega(E) = \int_{\Gamma} \delta(\mathcal{H}(p, q) - E) dpdq$$

is the density of states.

For our system of $N$ noninteracting particles in the volume $V$ we have:

$$\Omega(E) = \int_{\Gamma} \delta \left( \frac{|p|^2}{2m} - E \right) dpdq = V^N \int_{\{p \in \mathbb{R}^3N \mid |p| = \sqrt{2mE}\}} \frac{md\sigma}{|p|} = V^N (2mE)^{(3N-2)/2} S_{3N-1},$$

where

$$S_{3N-1} = \frac{2\pi^{3N/2}}{\Gamma(3N/2)}, \quad \Gamma(\cdot) \text{ is the gamma-function},$$
is the surface area of the unit $3N-1$-dimensional sphere embedded into $\mathbb{R}^{3N}$. Thus, the free energy is given by
\begin{equation}
\mu_H(E) = Z^{-1} V^{N} S_{3N-1} e^{-\beta E (2m E)} (3N-2)/2
\end{equation}

4. **Jarzynski’s equality**

Jarzynski’s equality (Christopher Jarzynski, Physics Professor in the University of Maryland, 1997) is the most significant result in the thermodynamics in the 20th century [3, 4, 5]. It relates the work performed by the system $W$ with the Helmholtz free energy change $\Delta F$ and replaces Clausius inequality $\langle W \rangle \geq \Delta F$. The equality in the Clausius inequality is achieved only if the process is isothermal and reversible (i.e., extremely slow). Jarzynski’s equality is valid for any kind of process, not necessarily reversible. It reads:
\begin{equation}
\langle e^{-W/k_B T} \rangle = e^{-\Delta F/k_B T},
\end{equation}
where $T$ is the initial temperature of the system and the thermal reservoir, and angular brackets denote ensemble average over realizations of the process.

**References**