

Classical Mechanics

Motion in \mathbb{R}^1

Let $x(t)$ denote position. Then, $v(t) = \frac{dx}{dt} = \dot{x}(t)$ is velocity (where the \cdot denotes derivative with respect to time), $a(t) = \dot{v}(t) = \ddot{x}(t)$, etc.

Considering Newton's second law, $F(x(t)) = m\ddot{x}(t)$, every exact solution requires initial conditions of $x(t_0)$ and $v(t_0)$. Solutions to Newton's second law are known as trajectories.

Considering a spring of constant k , $F(x) = -kx$ yields the differential equation $m\ddot{x} + kx = 0$. The general solution is

$$x(t) = a \cos(\omega t) + b \sin(\omega t),$$

with $\omega = \sqrt{k/m}$ denoting the frequency. The spring is an example of a simple harmonic oscillator.

Conservation of Energy

For a general force function $F(x)$, the kinetic energy is $\frac{1}{2}mv^2$, and the potential energy is

$$V(x) = - \int F(x) dx,$$

meaning $F(x) = -\frac{dV}{dx}$. The total energy is thus found as

$$E(x, v) = \frac{1}{2}mv^2 + V(x).$$

Proposition (Conservation of Energy). *If a particle with trajectory $x(t)$ satisfies $m\ddot{x} = F(x)$, then the energy E is conserved.*

Proof.

$$\begin{aligned} \frac{d}{dt} E(x(t), \dot{x}(t)) &= \frac{d}{dt} \left(\frac{1}{2}m(\dot{x}(t))^2 + V(x(t)) \right) \\ &= m\dot{x}(t)\ddot{x}(t) + \frac{dV}{dx}\dot{x}(t) \\ &= \dot{x}(t)(m\ddot{x}(t) - F(x(t))). \end{aligned}$$

□

By using the conservation of energy, we can reduce the second order differential equation $F(x) = m\ddot{x}$ to a system of first order differential equations in $x(t)$ and $v(t)$ respectively:

$$\begin{aligned} \frac{dx}{dt} &= v(t) \\ \frac{dv}{dt} &= \frac{1}{m}F(x(t)). \end{aligned}$$

If $(x(t), v(t))$ satisfies this set of equations, then $x(t)$ satisfies Newton's second law. We say the set of all possible (x, v) forms the phase space for the particle in \mathbb{R}^1 .

In phase space, conservation of energy implies that the set of all (x, v) must lie on the level curve of the energy function: $\{(x, v) \mid E(x, v) = E(x_0, v_0)\}$.

Using the conservation of energy, we find that, though Newton's second law is a second order differential equation in time, it is actually a first order differential equation:

$$\frac{m}{2} (\dot{x}(t))^2 + V(x(t)) = E(x(t_0), v(t_0))$$

$$\dot{x}(t) = \sqrt{\frac{2(E_0 - V(x(t)))}{m}}$$

Damping

Suppose we also introduce a force that depends on velocity — in the case of a damped simple harmonic oscillator, the equation for force changes from $F = -kx$ to $F = -kx - \gamma\dot{x}$, with $\gamma > 0$. The damping force acts in the opposite direction of velocity, meaning the particle slows down.

The equation of motion is then

$$m\ddot{x} + \gamma\dot{x} + kx = 0.$$

For γ small, the solutions are a sum sines and cosines multiplied by some exponential decay factor, but for γ large, the solutions are only the exponential decay.

Proposition (Energy Conservation in Damped Systems). *Suppose a particle moves along $x(t)$ that satisfies $F(x, \dot{x}) = F_1(x) - \gamma\dot{x}$, with $\frac{dV}{dx} = -F_1(x)$ and $\gamma > 0$. Then,*

$$\frac{d}{dt} E(x(t), \dot{x}(t)) = -\gamma\dot{x}(t)^2.$$

Proof.

$$\begin{aligned} \frac{d}{dt} E(x(t), \dot{x}(t)) &= \dot{x}(t) (m\ddot{x}(t) - F_1(x(t))) \\ &= \dot{x}(t) (m\ddot{x}(t) - (m\ddot{x}(t) + \gamma\dot{x}(t))) \\ &= -\gamma\dot{x}(t)^2 \end{aligned}$$

□

Motion in \mathbb{R}^n

The position of a particle $\mathbf{x} = (x_1, \dots, x_n)$ lends itself to velocity $\mathbf{v} = (v_1, \dots, v_n) = (\dot{x}_1, \dots, \dot{x}_n)$, and $\mathbf{a} = (\ddot{x}_1, \dots, \ddot{x}_n)$. Similar to in \mathbb{R}^1 , Newton's second law is denoted

$$m\ddot{\mathbf{x}} = \mathbf{F}(\mathbf{x}(t), \dot{\mathbf{x}}(t)).$$

Proposition (Conservation of Energy in n Dimensions). *The energy function*

$$E(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2} m \|\dot{\mathbf{x}}\|^2 + V(\mathbf{x})$$

is only satisfied where $\mathbf{F} = -\nabla V$.

Proof.

$$\begin{aligned} \frac{d}{dt} \left(\frac{1}{2} m \|\dot{\mathbf{x}}\|^2 + V(\mathbf{x}) \right) &= m \sum_{j=1}^n \dot{x}_j \ddot{x}_j + \sum_{j=1}^n \frac{\partial V}{\partial x_j} \dot{x}_j(t) \\ &= \dot{\mathbf{x}}(t) (m\ddot{\mathbf{x}}(t) + \nabla V) \\ &= \dot{\mathbf{x}}(t) (\mathbf{F}(\mathbf{x}) + \nabla V(\mathbf{x})), \end{aligned}$$

which is equal to zero only if $-\nabla V = \mathbf{F}$.

□

If \mathbf{F} is a smooth \mathbb{R}^n valued function on $U \subset \mathbb{R}^n$, then \mathbf{F} is conservative if there exists a smooth real-valued function V such that $\mathbf{F} = -\nabla V$.

In other words, \mathbf{F} is conservative if \mathbf{F} is a gradient field, implying that $\nabla \times \mathbf{F} = 0$.

If $\mathbf{F}(\mathbf{x}, \mathbf{y}) = -\nabla V(\mathbf{x}) + \mathbf{F}_2(\mathbf{x}, \mathbf{y})$, with $\mathbf{v} \cdot \mathbf{F}_2 = 0$ for all \mathbf{x} and \mathbf{v} , then energy is conserved along a given trajectory.

Systems of Particles

Let $\mathbf{x}^j = (x_1^j, x_2^j, \dots, x_n^j)$ denote the j th particle of a system of N particles. Newton's second law is thus reformulated as

$$m_j \ddot{\mathbf{x}}^j = \mathbf{F}^j(\mathbf{x}^1, \dots, \mathbf{x}^N, \dot{\mathbf{x}}^1, \dots, \dot{\mathbf{x}}^N).$$

The total energy is determined by

$$E(\mathbf{x}^1, \dots, \mathbf{x}^N, \mathbf{v}^1, \dots, \mathbf{v}^N) = \left(\sum_{j=1}^N \frac{1}{2} m_j \|\mathbf{v}^j\|^2 \right) + V(\mathbf{x}^1, \dots, \mathbf{x}^N).$$

Proposition (Conservation of Energy in a System of Particles). *The energy function is constant along each trajectory if $\nabla^j V = -\mathbf{F}^j$, where ∇^j denotes the gradient with respect to \mathbf{x}^j .*

The force function along a simply connected domain U in \mathbb{R}^{nN} satisfies $\nabla^j V = -\mathbf{F}^j$ if and only if

$$\frac{\partial F_k^j}{\partial x_m^l} = \frac{\partial F_m^l}{\partial x_k^j}$$

for all j, k, l, m .

Proof.

$$\begin{aligned} \frac{dE}{dt} &= \sum_{j=1}^N (m_j \dot{\mathbf{x}}^j \cdot \ddot{\mathbf{x}}^j + \nabla^j V \cdot \dot{\mathbf{x}}^j) \\ &= \sum_{j=1}^N \dot{\mathbf{x}}^j (m_j \ddot{\mathbf{x}}^j + \nabla^j V) \\ &= \sum_{j=1}^N \dot{\mathbf{x}}^j (\mathbf{F}^j + \nabla^j V), \end{aligned}$$

which is equal to zero if $\nabla^j V = -\mathbf{F}^j$.

Applying a higher dimension version of $\nabla \times \mathbf{F}$ to each coordinate pair (a, b) , we find the identity that shows \mathbf{F} is a gradient field. \square

Momentum of a System of Particles

The momentum of a particle \mathbf{p}^j is defined by

$$\mathbf{p}^j = m_j \dot{\mathbf{x}}^j.$$

Observe that $\frac{d\mathbf{p}^j}{dt} = m_j \ddot{\mathbf{x}}^j = \mathbf{F}^j$. The total momentum is then

$$\mathbf{p} = \sum_{j=1}^N \mathbf{p}^j.$$

Newton's third law, which states "for every action there is an equal and opposite reaction" applies if

- $\mathbf{F}^j = \sum_{k \neq j} \mathbf{F}^{j,k}(\mathbf{x}^j, \mathbf{y}^j);$
- $\mathbf{F}^{j,k}(\mathbf{x}_j, \mathbf{x}_k) = -\mathbf{F}^{k,j}(\mathbf{x}^k, \mathbf{x}^j).$

If each \mathbf{F}^j is also a conservative force, then satisfying these conditions yields potential energy in the form of

$$V(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N) = \sum_{j < k} V^{j,k}(\mathbf{x}^j - \mathbf{x}^k).$$

Proposition (Newton's Third Law and Conservation of Momentum). *If the system of particles satisfies the conditions of*

- $\mathbf{F}^j = \sum_{k \neq j} \mathbf{F}^{j,k}(\mathbf{x}^j, \mathbf{y}^j)$
- and $\mathbf{F}^{j,k}(\mathbf{x}_j, \mathbf{x}_k) = -\mathbf{F}^{k,j}(\mathbf{x}^k, \mathbf{x}^j),$

then total momentum is conserved.

Proof.

$$\begin{aligned} \frac{d\mathbf{p}}{dt} &= \sum_{j=1}^N \mathbf{F}^j \\ &= \sum_{j=1}^N \sum_{k \neq j} \mathbf{F}^{j,k}(\mathbf{x}^j, \mathbf{x}^k), \end{aligned}$$

and since $\mathbf{F}^{j,k}(\mathbf{x}^j, \mathbf{x}^k) + \mathbf{F}^{k,j}(\mathbf{x}^k, \mathbf{x}^j) = 0$, we find $\frac{d\mathbf{p}}{dt} = 0$. □

Proposition (Translation Invariance of Potential). *Let V denote the potential for a conservative force. Then, momentum is conserved if and only if V is translation invariant, meaning that for all $\mathbf{a} \in \mathbb{R}^n$,*

$$V(\mathbf{x}^1 + \mathbf{a}, \mathbf{x}^2 + \mathbf{a}, \dots, \mathbf{x}^N + \mathbf{a}) = V(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N).$$

Proof. Let $\mathbf{a} = t\mathbf{e}_k$. Then, differentiating at $t = 0$ with respect to t , we find

$$\begin{aligned} 0 &= \sum_{j=1}^N \frac{\partial V}{\partial x_k^j} \\ &= - \sum_{j=1}^N F_k^j \\ &= - \sum_{j=1}^N \frac{dp_k^j}{dt} \\ &= - \frac{dp_k}{dt}, \end{aligned}$$

with p_k denoting the k th component of \mathbf{p} . Therefore, \mathbf{p} is constant in time.

If \mathbf{p} is conserved, then the sum of all forces is 0 at each point for all t , meaning that for all t ,

$$\begin{aligned} \frac{d}{dt} V(\mathbf{x}^1 + t\mathbf{a}, \mathbf{x}^2 + t\mathbf{a}, \dots, \mathbf{x}^N + t\mathbf{a}) &= \sum_{j=1}^N \nabla^j V(\mathbf{x}^1 + t\mathbf{a}, \mathbf{x}^2 + t\mathbf{a}, \dots, \mathbf{x}^N + t\mathbf{a}) \cdot \mathbf{a} \\ &= - \left(\sum_{j=1}^N \mathbf{F}^j(\mathbf{x}^1 + t\mathbf{a}, \mathbf{x}^2 + t\mathbf{a}, \dots, \mathbf{x}^N + t\mathbf{a}) \right) \cdot \mathbf{a} \\ &= 0 \end{aligned}$$

meaning V is equal at $t = 0$ and $t = 1$. □

Center of Mass

For a system of N particles, the center of mass is denoted

$$\mathbf{c} = \sum_{j=1}^N \frac{m_j}{\sum_{j=1}^N m_j} \mathbf{x}_j.$$

We denote $\sum_{j=1}^N m_j = M$. Differentiating \mathbf{c} , we get

$$\begin{aligned} \frac{d\mathbf{c}}{dt} &= \frac{1}{M} \sum_{j=1}^N m_j \dot{\mathbf{x}}^j \\ &= \frac{\mathbf{p}}{M}. \end{aligned}$$

Notice that if \mathbf{p} is conserved, then $\mathbf{c}(t) = \mathbf{c}(t_0) + (t - t_0) \frac{\mathbf{p}}{M}$.

For a system of two particles, if $V(\mathbf{x}^1, \mathbf{x}^2)$ is invariant under translation, then $V(\mathbf{x}^1, \mathbf{x}^2) = \tilde{V}(\mathbf{x}^1 - \mathbf{x}^2)$, and $\tilde{V}(\mathbf{a}) = V(\mathbf{a}, 0)$.

The positions \mathbf{x}^1 and \mathbf{x}^2 can be recovered from knowledge about \mathbf{c} and the relative position $\mathbf{y} := \mathbf{x}^1 - \mathbf{x}^2$:

$$\begin{aligned} \mathbf{x}^1 &= \frac{\mathbf{c} + m_2 \mathbf{y}}{m_1 + m_2} \\ \mathbf{x}^2 &= \frac{\mathbf{c} - m_1 \mathbf{y}}{m_1 + m_2}. \end{aligned}$$

Thus, we can calculate

$$\begin{aligned} \ddot{\mathbf{y}} &= \ddot{\mathbf{x}}^1 - \ddot{\mathbf{x}}^2 \\ &= -\frac{1}{m_1} \nabla \tilde{V}(\mathbf{x}^1 - \mathbf{x}^2) - \frac{1}{m_2} \nabla \tilde{V}(\mathbf{x}^1 - \mathbf{x}^2). \end{aligned}$$

Motion of Relative Position under Translation Invariant Potential

For a two particle system with translation invariant potential, the relative position $\mathbf{y} = \mathbf{x}^1 - \mathbf{x}^2$ is a solution to the differential equation

$$\mu \ddot{\mathbf{y}} = -\nabla \tilde{V}(\mathbf{y}),$$

where

$$\mu = \frac{m_1 m_2}{m_1 + m_2}.$$

This implies that when momentum is conserved, the relative position of the two particle system evolves as a one-particle system with effective mass μ .

Angular Momentum

A particle moving in \mathbb{R}^2 with position \mathbf{x} , velocity \mathbf{v} , and momentum $\mathbf{p} = m\mathbf{v}$ has angular momentum J denoted as

$$J = x_1 p_2 - x_2 p_1,$$

or $J = \|\mathbf{x} \times \mathbf{p}\| = \|\mathbf{x}\| \|\mathbf{p}\| \sin \phi$, with ϕ measured counterclockwise. In polar coordinates, we find

$$\begin{aligned} J &= mr^2 \frac{d\theta}{dt} \\ &= 2M \frac{dA}{dt}, \end{aligned}$$

where $A = 1/2 \int r^2 d\theta$ denotes the area swept out by $\mathbf{x}(t)$.

Proposition (Conservation of Angular Momentum). *Suppose a particle of mass m is moving in \mathbb{R}^2 under the influence of a conservative force with potential $V(\mathbf{x})$. V is invariant under rotation if and only if J is conserved.*

Proof.

$$\begin{aligned} \frac{dJ}{dt} &= \frac{dx_1}{dt} p_2 + x_1 \frac{dp_2}{dt} - \frac{dx_2}{dt} p_1 - x_2 \frac{dp_1}{dt} \\ &= \frac{1}{m} p_1 p_2 - x_1 \frac{\partial V}{\partial x_2} - \frac{1}{m} p_2 p_1 + x_2 \frac{\partial V}{\partial x_1} \\ &= x_2 \frac{\partial V}{\partial x_1} - x_1 \frac{\partial V}{\partial x_2}. \end{aligned}$$

Alternatively, consider $R_\theta = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$. Differentiating V along R_θ , we get

$$\begin{aligned} \left. \frac{d}{d\theta} V(R_\theta \mathbf{x}) \right|_{\theta=0} &= \frac{\partial V}{\partial x} \frac{dx}{d\theta} + \frac{\partial V}{\partial y} \frac{dy}{d\theta} \\ &= -x_2 \frac{\partial V}{\partial x_1} + x_1 \frac{\partial V}{\partial x_2} \\ &= -\frac{dJ}{dt}(\mathbf{x}) \end{aligned}$$

Thus, $\frac{dJ}{dt} = 0$ if and only if the angular derivative of V is zero. □

As a result of the conservation of angular momentum, we thus get Kepler's Second Law: if $\mathbf{x}(t)$ is the trajectory of a particle under the influence of a force with rotationally invariant potential, then the area swept out by $\mathbf{x}(t)$ between $t = a$ and $t = b$ is $\frac{b-a}{2m} J$.

In \mathbb{R}^3 , \mathbf{J} is a vector given by $\mathbf{x} \times \mathbf{p}$. Meanwhile, in \mathbb{R}^n , the angular momentum is a skew-symmetric matrix defined by

$$J_{jk} = x_j p_k - x_k p_j.$$

The total angular momentum of a system of N particles in \mathbb{R}^n is given by \mathbf{J} with entries

$$J_{jk} = \sum_{l=1}^N (x_j^l p_k^l - x_k^l p_j^l).$$

Similar to the case of linear momentum, angular momentum is constant in the presence of a conservative force if and only if the potential function V is rotationally invariant. That is,

$$V(R\mathbf{x}^1, R\mathbf{x}^2, \dots, R\mathbf{x}^N) = V(\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N)$$

for all rotation matrices R .

Hamiltonian Mechanics

The Hamiltonian is the total energy function, but formulated in terms of position and momentum rather than position and velocity. If a particle in \mathbb{R}^n has the usual energy function, we write

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m} \sum_{j=1}^n p_j^2 + V(\mathbf{x}),$$

where $p_j = m_j \dot{x}_j$. Observe that the equations of motion can be written as

$$\begin{aligned} \frac{dx_j}{dt} &= \frac{\partial H}{\partial p_j} \\ \frac{dp_j}{dt} &= -\frac{\partial H}{\partial x_j}. \end{aligned}$$

In the basic formulation, we can see that the first equation is just $\dot{x}_j = p_j/m$, and $\dot{p}_j = F_j$. The equations of motion written with Hamiltonians are known as Hamilton's equations.

Poisson Bracket

Let f and g be two smooth functions on \mathbb{R}^{2n} , with each element of \mathbb{R}^{2n} being denoted by (\mathbf{x}, \mathbf{p}) . The Poisson bracket of f and g is equal to

$$\{f, g\}(\mathbf{x}, \mathbf{p}) = \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial x_j} \right).$$

The Poisson bracket satisfies the following properties:

- Linearity: $\{f, g + ch\} = \{f, g\} + c\{f, h\}$
- Antisymmetry: $\{g, f\} = -\{f, g\}$
- Product Rule: $\{f, gh\} = \{f, g\}h + g\{f, h\}$
- Jacobi Identity: $\{f, \{g, h\}\} + \{h, \{f, g\}\} + \{g, \{h, f\}\} = 0$.

It can be easily verified that the following Poisson bracket relations hold:

$$\begin{aligned} \{x_j, x_k\} &= 0 \\ \{p_j, p_k\} &= 0 \\ \{x_j, p_k\} &= \delta_{jk}, \end{aligned}$$

where δ_{jk} denotes the Kronecker delta function.

Proposition (Solutions of Hamilton's Equations). *If $(\mathbf{x}(t), \mathbf{p}(t))$ is a solution to Hamilton's Equations, then for any smooth f on \mathbb{R}^{2n} , we have*

$$\frac{df}{dt} = \{f, H\}.$$

Proof.

$$\begin{aligned} \frac{df}{dt} &= \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{dx_j}{dt} + \frac{\partial f}{\partial p_j} \frac{dp_j}{dt} \right) \\ &= \sum_{j=1}^n \left(\frac{\partial f}{\partial x_j} \frac{\partial H}{\partial p_j} + \frac{\partial f}{\partial p_j} \left(-\frac{\partial H}{\partial x_j} \right) \right) \\ &= \{f, H\}. \end{aligned}$$

□

Conserved Quantities

Let $f \in C^1(\mathbb{R}^{2n})$ be called conserved if $f(\mathbf{x}(t), \mathbf{p}(t))$ is independent of t for each solution to Hamilton's equation. Then, f is a conserved quantity if and only if

$$\{f, H\} = 0.$$

Note that H is also a conserved quantity.

Flow and Liouville's Theorem

Solving Hamilton's equations on \mathbb{R}^{2n} yields a flow Φ_t^1 with $\Phi_t(\mathbf{x}, \mathbf{p})$ equal to the solution at time t with initial condition (\mathbf{x}, \mathbf{p}) .

The Φ_t aren't necessarily defined on all of \mathbb{R}^{2n} , but if Φ_t is defined on \mathbb{R}^{2n} for all t , then we say Φ_t is complete.

Proposition (Liouville²). *The Hamiltonian flow preserves the $2n$ -dimensional measure.*

$$dx_1 dx_2 \cdots dx_n dp_1 dp_2 \cdots dp_n.$$

More specifically, if E is a measurable subset of the domain of Φ_t , then $\mu(\Phi_t(E)) = \mu(E)$.

Proof. Hamilton's equations can be written as

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ \vdots \\ x_n \\ p_1 \\ \vdots \\ p_n \end{bmatrix} = \begin{bmatrix} \frac{\partial H}{\partial p_1} \\ \vdots \\ \frac{\partial H}{\partial p_n} \\ -\frac{\partial H}{\partial x_1} \\ \vdots \\ -\frac{\partial H}{\partial x_n} \end{bmatrix}.$$

Hamilton's equations describe the flow along the vector field appearing on the right side — by a result in vector calculus,³ the flow preserves the $2n$ -dimensional area measure if and only if the divergence of the vector field is zero.

$$\begin{aligned} \nabla \cdot \begin{bmatrix} \frac{\partial H}{\partial p_1} \\ \vdots \\ \frac{\partial H}{\partial p_n} \\ -\frac{\partial H}{\partial x_1} \\ \vdots \\ -\frac{\partial H}{\partial x_n} \end{bmatrix} &= \sum_{k=1}^n \frac{\partial}{\partial x_k} \frac{\partial H}{\partial p_k} - \frac{\partial}{\partial p_k} \frac{\partial H}{\partial x_k} \\ &= \sum_{k=1}^n \frac{\partial^2 H}{\partial x_k \partial p_k} - \frac{\partial^2 H}{\partial p_k \partial x_k} \\ &= 0 \end{aligned}$$

□

The condition of zero divergence is equivalent to Φ_t preserving a particular symplectic form ω defined by

$$\omega((\mathbf{x}, \mathbf{p}), (\mathbf{x}', \mathbf{p}')) = \mathbf{x} \cdot \mathbf{p}' - \mathbf{p} \cdot \mathbf{x}',$$

¹the Φ_t are diffeomorphisms, or differentiable isomorphisms with differentiable inverses

²not from complex analysis

³Author's Note: I do not know this result yet, but hopefully I will soon!

meaning that for any t and any $(\mathbf{x}, \mathbf{p}) \in \mathbb{R}^{2n}$, the partial derivatives of Φ_t preserves ω .

Alternatively, this is equivalent to Φ_t preserving Poisson brackets:

$$\{f \circ \Phi_t, g \circ \Phi_t\} = \{f, g\} \circ \Phi_t.$$

Thus, Φ_t is an example of a symplectomorphism.

Hamiltonian Flow and Hamiltonian Generators

We say $f \in C^1(\mathbb{R}^{2n})$ is the Hamiltonian generator of the flow that results from solving Hamilton's equations with f substituted for H :

$$\begin{aligned} \frac{dx_j}{dt} &= \frac{\partial f}{\partial p_j} \\ \frac{dp_j}{dt} &= -\frac{\partial f}{\partial x_j}. \end{aligned}$$

It is possible to see that

$$f_a(\mathbf{x}, \mathbf{p}) = \mathbf{a} \cdot \mathbf{p}$$

yields the flow

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}_0 + t\mathbf{a} \\ \mathbf{p}(t) &= \mathbf{p}_0, \end{aligned}$$

and

$$g_b(\mathbf{x}, \mathbf{p}) = \mathbf{b} \cdot \mathbf{x}$$

yields the flow

$$\begin{aligned} \mathbf{x}(t) &= \mathbf{x}_0 \\ \mathbf{p}(t) &= \mathbf{p}_0 - t\mathbf{b}. \end{aligned}$$

Thus, the Hamiltonian flow generated by momentum yields translation in position, and the Hamiltonian flow generated by position yields translation in momentum.

In this light, we can think of *the* Hamiltonian as the Hamiltonian generator that yields time evolution. Other Hamiltonian generators represent some other family of symmetries of the system.

Proposition (Hamiltonian Flow generated by Angular Momentum). *For a particle moving in \mathbb{R}^2 , the Hamiltonian flow generated by*

$$J(\mathbf{x}, \mathbf{p}) = x_1 p_2 - x_2 p_1$$

consists of simultaneous rotations of \mathbf{x} and \mathbf{p} .

$$\begin{aligned} \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} &= \begin{bmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{bmatrix} \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix} \\ \begin{bmatrix} p_1(t) \\ p_2(t) \end{bmatrix} &= \begin{bmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{bmatrix} \begin{bmatrix} p_1(0) \\ p_2(0) \end{bmatrix}. \end{aligned}$$

Proof. Plugging J Hamilton's equations, we get

$$\begin{aligned}\frac{dx_1}{dt} &= \frac{\partial J}{\partial p_1} = -x_2 \\ \frac{dp_1}{dt} &= -\frac{\partial J}{\partial x_1} = -p_2 \\ \frac{dx_2}{dt} &= \frac{\partial J}{\partial p_2} = x_1 \\ \frac{dp_2}{dt} &= -\frac{\partial J}{\partial x_2} = p_1.\end{aligned}$$

□

It's important to note that the parameter t in the Hamiltonian flow for J is the rotation, not time. That is, J is the Hamiltonian generator of rotations.

If f is any smooth function, it is the case that the time derivative of any other function g along the Hamiltonian flow generated by f is $\frac{dg}{dt} = \{g, f\}$. In particular, the derivative of H along the flow generated by f is $\{H, f\}$, meaning that f is constant along the flow generated by H if and only if $\{f, H\} = 0$, which is true if and only if H is constant along the flow generated by H .

Thus, we find that f is conserved for solutions of Hamilton's equations if and only if H is invariant under the Hamiltonian flow generated by f . Of particular note, we find that J is conserved if and only if H is invariant under rotations of \mathbf{x} and \mathbf{p} .⁴

Introduction to Quantum Mechanics

Observable quantities such as position and momentum in quantum mechanics are represented by operators on a complex-valued Hilbert space (an inner product space that is complete with respect to the induced metric) — specifically, these quantities are *unbounded* linear operators.

In physics, the inner product is linear in the second factor and conjugate linear in the first factor:

$$\begin{aligned}\langle \phi, \lambda \psi \rangle &= \lambda \langle \phi, \psi \rangle \\ \langle \lambda \phi, \psi \rangle &= \overline{\lambda} \langle \phi, \psi \rangle.\end{aligned}$$

Alternatively, in Dirac notation:

$$\begin{aligned}\langle \phi | \lambda \psi \rangle &= \lambda \langle \phi | \psi \rangle \\ \langle \lambda \phi | \psi \rangle &= \overline{\lambda} \langle \phi | \psi \rangle.\end{aligned}$$

A Taste of Operator Theory

A linear operator $A : \mathbf{H} \rightarrow \mathbf{H}$ is bounded if it has finite operator norm:⁵

$$\sup_{\|\psi\| \leq 1} \|A\psi\| < \infty.$$

For each bounded operator A , there exists a unique bounded operator A^* such that $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$. The existence of A^* follows from the Riesz representation theorem.

⁴There is another section on Kepler's Laws in the chapter on Classical Mechanics that I didn't really read in depth. I might include it in the future.

⁵I'm using more operator-theoretic language than the book uses because I'm ~~pretentious~~ a mathematician, not a physicist.

A bounded operator is said to be self-adjoint if $A^* = A$. Self-adjoint operators are nice for a variety of reasons, and as a result we desire for our operators in quantum mechanics to be self-adjoint. However, this brings a significant problem — unbounded self-adjoint operators are not necessarily defined on \mathbf{H} .

We define unbounded operators as linear operators defined on a dense subspace of \mathbf{H} :

$$A : \text{Dom}(A) \subseteq \mathbf{H} \rightarrow \mathbf{H}$$

subject to

$$\overline{\text{Dom}(A)} = \mathbf{H}.$$

In addition to the domain of A not necessarily being equal to \mathbf{H} , the linear functional $\langle \phi, A \cdot \rangle$ is not necessarily bounded (meaning we cannot use the Riesz representation theorem to find $A^* \phi$). The adjoint of A , as a result, will be defined on a subspace of \mathbf{H} .

A vector $\phi \in \mathbf{H}$ is said to belong to the domain $\text{Dom}(A^*)$ if the linear functional $\langle \phi, A \cdot \rangle$ on $\text{Dom}(A)$ is bounded. Then, we define A^* to be the unique vector χ such that $\langle \chi, \psi \rangle = \langle \phi, A\psi \rangle$ for all $\psi \in \text{Dom}(A)$.

Having defined adjoints of an unbounded operator, we can now commit to defining self-adjoint operators. The operator A is symmetric if $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ — a symmetric operator is self-adjoint if $\text{Dom}(A) = \text{Dom}(A^*)$ and $A^* \phi = A\phi$ for all $\phi \in \text{Dom}(A)$. Finally, A is essentially self-adjoint if the closure of the graph of A in $\mathbf{H} \times \mathbf{H}$ is self-adjoint.

In sum, A is self-adjoint if A and A^* are the same operator with the same domain, more or less.

Definition (Properties of Symmetric Operators). Let A be a symmetric operator on \mathbf{H} . Then, the following hold:

- (1) For all $\psi \in \text{Dom}(A)$, the quantity $\langle \psi, A\psi \rangle$ is real. More generally, if $\psi, A\psi, \dots, A^{m-1}\psi$ belong to $\text{Dom}(A)$, then $\langle \psi, A^m \psi \rangle$ is real.
- (2) Suppose λ is an eigenvector for A . Then, $\lambda \in \mathbb{R}$.

Proof. (1) Since A is symmetric,

$$\begin{aligned} \langle \psi, A\psi \rangle &= \langle A\psi, \psi \rangle \\ &= \overline{\langle \psi, A\psi \rangle}, \end{aligned}$$

for all $\psi \in \text{Dom}(A)$. Similarly, if $\psi, A\psi, \dots, A^{m-1}\psi \in \text{Dom}(A)$, then we use the symmetry of A to show that

$$\begin{aligned} \langle \psi, A^m \psi \rangle &= \langle A^m \psi, \psi \rangle \\ &= \overline{\langle \psi, A^m \psi \rangle}. \end{aligned}$$

- (2) If ψ is an eigenvector for A with eigenvalue λ , then

$$\begin{aligned} \lambda \langle \psi, \psi \rangle &= \langle \psi, A\psi \rangle \\ &= \langle A\psi, \psi \rangle \\ &= \bar{\lambda} \langle \psi, \psi \rangle. \end{aligned}$$

Since ψ is nonzero by definition, it must be the case that $\lambda = \bar{\lambda}$.

□

In physical terms, $\langle \psi, A\psi \rangle$ represents the expected value for measurements of A in the state ψ , with λ representing a possible value of this measurement. This is why we want both numbers to be real.

A self-adjoint A allows us to use the spectral theorem to assign each $\psi \in \mathbf{H}$ a probability measure on the real numbers.

Position and Momentum Operators

Consider a particle moving along the real line with wave function $\psi : \mathbb{R} \rightarrow \mathbb{C}$. Although ψ will evolve over time, let the particle be fixed in time for now.

We want to define ψ to be a unit vector in $L^2(\mathbb{R})$, meaning

$$\int_{\mathbb{R}} |\psi(x)|^2 dx = 1.$$

The probability that the position of the particle belongs to some $E \subseteq \mathbb{R}$ is

$$\int_E |\psi(x)|^2 dx,$$

where E is necessarily a Lebesgue-measurable set.

The expectation value of the position is thus

$$E(x) = \int_{\mathbb{R}} x |\psi(x)|^2 dx,$$

assuming the convergence of the integral, and the m th moment of the position is calculated as

$$E(x^m) = \int_{\mathbb{R}} x^m |\psi(x)|^2 dx,$$

again assuming convergence of the integral.

Definition (Position Operator). The position operator is defined as $X = M_x$, meaning $(X\psi)(x) = x\psi(x)$. With this in mind, we can then see that

$$E(x) = \langle \psi, X\psi \rangle$$

under the standard inner product on $L^2(\mathbb{R})$. The expectation value of X for the state ψ is denoted $\langle X \rangle_{\psi} := \langle \psi, X\psi \rangle$.⁶

The higher moments of position are similarly defined:

$$E(x^m) = \langle \psi, X^m \psi \rangle,$$

where X^m denotes m -degree composition of X .

Since X is an unbounded linear operator, it is not necessarily the case that $X\psi \in L^2(\mathbb{R})$ if $\psi \in L^2(\mathbb{R})$.⁷

Momentum is encoded in the oscillations of the wave function — the de Broglie hypothesis provides a special relationship between the frequency of oscillation (as a function of position at a fixed time) and the momentum.

Proposition (De Broglie Hypothesis). *If the wave function of a particle has angular frequency k , then the momentum p of the particle is*

$$p = \hbar k,$$

where \hbar denotes Planck's constant.

⁶I don't like this notation either.

⁷Other famous examples of unbounded linear operators on Hilbert spaces include the derivative operator on $A^2(\mathbb{D})$, the space of holomorphic functions on the complex unit disc. I'm doing research on properties of variations of this space.

To be more precise, the de Broglie hypothesis applies to wave functions of the form $\psi(x) = e^{ikx}$, which represents particles that have momentum $p = \hbar k$. Let's develop this a bit further.

Since e^{ikx} is not square integrable over \mathbb{R} , we instead move to the circle, where ψ has period 2π over \mathbb{R} , and

$$\int_0^{2\pi} |\psi(x)|^2 dx = 1.$$

For any integer k , the normalized wave function $\frac{e^{ikx}}{\sqrt{2\pi}}$ will represent the particle with momentum $p = \hbar k$. This momentum value is definite; that is, $p = \hbar k$ with probability 1 for a particle with wave function $\frac{e^{ikx}}{\sqrt{2\pi}}$.

Of note, the functions $\left\{ \frac{e^{ikx}}{\sqrt{2\pi}} \right\}$ for $k \in \mathbb{Z}$ form an orthonormal basis for the Hilbert space of square integrable functions with period 2π .

The wave functions for particles on a circle are thus all of the form

$$\psi(x) = \sum_{k=-\infty}^{\infty} a_k \frac{e^{ikx}}{\sqrt{2\pi}},$$

where the sum is convergent in $L^2([0, 2\pi])$.⁸ If ψ is a unit vector, then⁹

$$\begin{aligned} \|\psi\|_{L^2([0, 2\pi])}^2 &= \sum_{k=-\infty}^{\infty} |a_k|^2 \\ &= 1. \end{aligned}$$

For a particle with wave function ψ expressed as a Fourier series, the momentum isn't definite. We will have to consider that measurement will yield one of the values of $\hbar k$ with probability $|a_k|^2$.

$$E(p) = \sum_{k=-\infty}^{\infty} \hbar k |a_k|^2,$$

with higher moments defined by

$$E(p^m) = \sum_{k=-\infty}^{\infty} (\hbar k)^m |a_k|^2,$$

assuming absolute convergence.

Definition (Momentum Operator). To encode P , our momentum operator, such that for the wave function $\psi \in L^2([0, 2\pi])$, $E(p^m) = \langle \psi, P^m \psi \rangle$, we must have P satisfying

$$P e^{ikx} = \hbar k e^{ikx}.$$

Thus, we would assume that

$$P = -i\hbar \frac{d}{dx}.$$

Even on the real line, we would still expect $P = -i\hbar \frac{d}{dx}$; though e^{ikx} is not square integrable, we can represent any wave function $\psi \in L^2(\mathbb{R})$ as an integral with the Fourier transform:

$$\begin{aligned} \psi(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ikx} \hat{\psi}(k) dk, \\ \hat{\psi}(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \psi(x) dx. \end{aligned}$$

⁸You may recognize these as Fourier series.

⁹We use Parseval's identity to relate the L^2 norm of ψ to the ℓ^2 norm of $\{a_k\}_{k \in \mathbb{Z}}$. Try proving it yourself! Hint: use the Pythagorean theorem.

Plancherel's theorem¹⁰ states that the Fourier transform is unitary — that is,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} |\hat{\psi}(k)|^2 dk = 1.$$

We can imagine $\hat{\psi}(k)$ as the probability density for the momentum of the particle¹¹.

Thus, we have defined the momentum operator as

$$P = -i\hbar \frac{d}{dx},$$

with, for sufficiently nice $\psi \in L^2(\mathbb{R})$

$$\begin{aligned} E(p^m) &= \langle \psi, P^m \psi \rangle \\ &= \int_{-\infty}^{\infty} (\hbar k)^m |\hat{\psi}(k)|^2 dk \end{aligned}$$

for all positive integers m .

Proposition (Commutator of Position and Momentum).

$$[X, P] = i\hbar I,$$

a relation known as the canonical commutation relation.

Proof.

$$\begin{aligned} PX\psi &= -i\hbar \frac{d}{dx} (x\psi(x)) \\ &= -i\hbar \psi(x) - i\hbar x \frac{d\psi}{dx} \\ &= -i\hbar I\psi + XP\psi \end{aligned}$$

□

Remark. Note the parallel between $\{x, p\} = 1$ in the Poisson bracket and $[X, P] = i\hbar I$ in the commutator.

Proposition (Symmetry of Position and Momentum Operators). For all sufficiently nice ϕ and ψ in $L^2(\mathbb{R})$,

$$\begin{aligned} \langle \phi, X\psi \rangle &= \langle X\phi, \psi \rangle \\ \langle \phi, P\psi \rangle &= \langle P\phi, \psi \rangle. \end{aligned}$$

Proof. Let $\phi, \psi \in L^2(\mathbb{R})$ with $x\psi(x), x\phi(x) \in L^2(\mathbb{R})$. Then, since $x \in \mathbb{R}$,

$$\int_{-\infty}^{\infty} \overline{\phi(x)} x\psi(x) dx = \int_{-\infty}^{\infty} \overline{x\phi(x)} \psi(x) dx,$$

with both integrals convergent.

Meanwhile, assume ϕ and ψ are continuously differentiable, vanish at $\pm\infty$, and $\phi, \psi, \frac{d\phi}{dx}, \frac{d\psi}{dx} \in L^2(\mathbb{R})$. Note that $\frac{d\bar{\phi}}{dx} = \overline{\frac{d\phi}{dx}}$. Then, integrating by parts,

$$-i\hbar \int_{-n}^n \overline{\phi(x)} \frac{d\psi}{dx} dx = -i\hbar \overline{\phi(x)} \psi(x) \Big|_{-n}^n + i\hbar \int_{-n}^n \frac{d\bar{\phi}}{dx} \psi(x) dx,$$

¹⁰also known as Parseval's theorem when applied to Fourier series rather than the Fourier transform

¹¹well, for p/\hbar , but that's basically the same

meaning

$$\begin{aligned}\int_{-\infty}^{\infty} \overline{\phi(x)} \left(-i\hbar \frac{d\psi}{dx} \right) dx &= i\hbar \int_{-\infty}^{\infty} \overline{\frac{d\phi}{dx}} \psi(x) dx \\ &= \int_{-\infty}^{\infty} \overline{\left(-i\hbar \frac{d\phi}{dx} \right)} \psi(x) dx.\end{aligned}$$

□

Thus, we have shown that X and P are symmetric operators on certain dense subspaces of $L^2(\mathbb{R})$. We will have to wait until later to prove that X and P are essentially self-adjoint.