A Primer in Quantum Mechanics

Ross Dempsey

Revised September 17, 2018

"If you have built castles in the air, your work need not be lost; that is where they should be. Now put the foundations under them." – Henry David Thoreau

Abstract

There are plenty of introductions to quantum physics, and there is little need for another which takes a standard approach. The aim of these notes is to provide an alternative entry point into quantum theory. The focus is on quantization, in order to make as apparent as possible the origins of a quantum theory out of a classical one. However, since this is meant as an introduction, it is not a sophisticated presentation of any rigorous quantization scheme (though it mostly follows canonical quantization). It might be called "intuitive quantization," owing to the focus on building a deep physical understanding of the quantum state space and the operators acting on it.

Contents

1 Classical Theory

A first presentation of Newtonian mechanics will invariably start with Newton's second law,

$$\boldsymbol{F} = m\boldsymbol{a}.$$

With this law, and knowledge of the forces between objects, classical mechanics is immediately reduced to systems of differential equations. The physics of classical mechanics could end here, and anyone interested in physical predictions could be handed the information sheet for Mathematica's `NDSolve` routine. This, of course, would be a travesty. There is a great deal more physics than Newton's second law would suggest, such as conservation laws for energy, momentum, and angular momentum. A formal ability to solve for the dynamics of a system, while desirable, is not at all equivalent to a physical understanding of the system.

Aware of this deficit in Newton's laws, we will construct the Lagrangian formulation of mechanics, which has the advantage of making conservation laws into manifest consequences of symmetries. We will then move to the Hamiltonian formulation, in which the reverse connection is made apparent by conserved quantities generating their associated symmetries.

1.1 Lagrangian Mechanics

The idea of an *action principle* began with Maupertuis in the mid-18$^{\text{th}}$ century. He noted that, in the motion of a point particle, the product of mass, velocity, and distance is minimized. He referred to this product as the *action* of the motion. Maupertuis's motivation was largely to find fingerprints of God in the basic physical laws, and he believed that his result constituted undeniable proof of a heavenly design. Few would agree today, but we will find that an action principle can be deeply informative in other ways.

First, we will attempt to find reasoning behind Maupertuis's principle. Consider a particle of mass m moving along a line from a to b. If it is moving at a constant velocity v, then Maupertuis's action would be $S \equiv mv(b-a)$. However, it may move at different velocities over different intervals, so more generally we should write

$$S \equiv \sum_{i=1}^{n} mv_i(b_i - a_i) \qquad (a_1 = a, b_n = b).$$

If the velocity is continuously changing, then we pass to the limit $n \to \infty$ and recognize the expression as a Riemann sum for the integral

$$S \equiv \int_a^b mv(x)\,dx.$$

Since velocity is more likely to be known as a function of time than as a function of position, it is wise at this point to rewrite the integral as an integral over time. Using $v = \frac{dx}{dt}$, we find

$$S \equiv \int_{t_a}^{t_b} mv^2\,dt.$$

This expression is already interesting – the kinetic energy has appeared in the integrand. The next question is what it means for this quantity to be minimized. If we had only one parameter for a function to be minimized, we could simply take a derivative with respect to that parameter and require it to vanish. If there were n parameters in a vector, we would require the derivative in any direction to vanish. This amounts to requiring

$$\frac{d}{d\epsilon} S(\boldsymbol{x} + \epsilon \boldsymbol{\eta}) \bigg|_{\epsilon=0} = 0$$

for all directions $\boldsymbol{\eta}$. When we manipulate this expression we obtain the condition $\boldsymbol{\eta} \cdot \boldsymbol{\nabla} S = 0$, and in order for this to be satisfied for arbitrary $\boldsymbol{\eta}$, it must be the case that $\boldsymbol{\nabla} S = 0$.

In our case, we have not one or a finite number of parameters, but an infinite number. Our parameter is the trajectory $x(t)$ (and its derivative $v(t) = \dot{x}(t)$, which enters directly into the Maupertuis action). We will follow a procedure analogous to the one for a vector of parameters: require the derivative to vanish in any direction. The condition is

$$\frac{d}{d\epsilon} S[x(t) + \epsilon \eta(t)] \bigg|_{\epsilon=0} = 0.$$

By substituting $x(t) + \epsilon\eta(t)$ into the expression for action, we obtain

$$\frac{d}{d\epsilon} \left(\int_{t_a}^{t_b} m(\dot{x}(t) + \epsilon \dot{\eta}(t))^2 \, dt \right)_{\epsilon=0} = 0.$$

Moving the derivative through the integral, this becomes

$$2m \int_{t_a}^{t_b} \dot{x}(t)\dot{\eta}(t) \, dt = -2m \int_{t_a}^{t_b} \ddot{x}(t)\eta(t) \, dt = 0,$$

where the first equality is an integration by parts (and we assume $\eta(t_a) = \eta(t_b) = 0$). This can only be satisfied for arbitrary $\eta(t)$ if $\ddot{x}(t) = 0$ identically, which is indeed the correct prediction for a free particle. Note also that if we had treated the mass as a dynamical variable, we would find $\frac{d}{dt}(mv) = 0$, again the correct prediction.

This idea can be generalized to encapsulate all modern theories of physics. By changing the integrand in the action, which is called the *Lagrangian*, we change the resulting equations of motion. It is very helpful to be able to go directly from a Lagrangian to its equations of motion, so we will derive the equations of motion for a general case. Let the action be given by

$$S[x(t)] = \int_{t_a}^{t_b} \mathcal{L}(x(t), \dot{x}(t)) \, dt,$$

where $\mathcal{L}$ is the Lagrangian. If S is stationary, it must be the case that

$$\frac{d}{d\epsilon} S[x(t) + \epsilon \eta(t)] \bigg|_{\epsilon=0} = 0$$

for any $\eta(t)$ satisfying $\eta(t_a) = \eta(t_b) = 0$. This derivative is

$$0 = \frac{d}{d\epsilon} S[x(t) + \epsilon \eta(t)] \bigg|_{\epsilon=0} = \int_{t_a}^{t_b} \left(\frac{\partial \mathcal{L}}{\partial x} \eta(t) + \frac{\partial \mathcal{L}}{\partial \dot{x}} \dot{\eta}(t) \right) \, dt.$$

Integrating by parts in the second term, we have

$$0 = \int_{t_a}^{t_b} \left(\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} \right) \eta(t)\, dt.$$

Since this must hold for any $\eta(t)$, it follows that

$$\frac{\partial \mathcal{L}}{\partial x} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}} = 0.$$

This is called the *Euler-Lagrange equation*. When we apply it to the Maupertuis action, with $\mathcal{L} = m\dot{x}^2$, we find $\frac{d}{dt}(m\dot{x}) = 0$. In order to obtain Newton's second law with a nonzero force, we need a force to appear on the right hand side of this expression. Since a conservative force is given by $F = -\frac{\partial V}{\partial x}$, where $\frac{\partial V}{\partial \dot{x}} = 0$, we can use the $\frac{\partial \mathcal{L}}{\partial x}$ term in the Euler-Lagrange equation to add a force. Indeed, if we choose $\mathcal{L} = \frac{1}{2}m\dot{x}^2 - V(x) = T - V$, where T is the kinetic energy, the Euler-Lagrange equation is

$$\frac{d}{dt}(m\dot{x}) = -\frac{dV}{dx}.$$

If we have a particle moving through more than one dimension, the action must be stationary for perturbations in any direction in space. This means the Euler-Lagrange equations must be satisfied for every coordinate:

$$\frac{\partial \mathcal{L}}{\partial x^i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}^i} = 0.$$

Intuitively, this result is not specific to Cartesian coordinates; it should hold even if we work in a curvilinear coordinate system. The key fact is that perturbations of a path in any coordinate direction, whatever those coordinates are chosen to be, should leave the action stationary. To prove this formally, we will demonstrate that the quantities

$$\alpha_i = \frac{\partial \mathcal{L}}{\partial x^i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}^i}$$

form a vector. In fact, they form a covariant vector, or a type (0,1) tensor. To prove this, we must take an arbitrary coordinate transformation $x^i = x^i(\tilde{x}^j)$, and establish that the α_i obey the transformation law

$$\tilde{\alpha}_i = \frac{\partial x^j}{\partial \tilde{x}^i}\alpha_j.$$

Using the chain rule, we have

$$\frac{\partial \mathcal{L}}{\partial \tilde{x}^i} = \frac{\partial \mathcal{L}}{\partial x^j}\frac{\partial x^j}{\partial \tilde{x}^i} + \frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{\partial \dot{x}^j}{\partial \tilde{x}^i},$$
$$\frac{\partial \mathcal{L}}{\partial \dot{\tilde{x}}^i} = \frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{\partial \dot{x}^j}{\partial \dot{\tilde{x}}^i}.$$

Since

$$\dot{x}^i = \frac{dx^i}{dt} = \frac{\partial x^i}{\partial \tilde{x}^j}\dot{\tilde{x}}^j + \frac{\partial x^i}{\partial t},$$

we have

$$\frac{\partial \dot{x}^i}{\partial \dot{\tilde{x}}^j} = \frac{\partial x^i}{\partial \tilde{x}^j}$$

and

$$\frac{\partial \dot{x}^i}{\partial \tilde{x}^j} = \frac{\partial}{\partial \tilde{x}^k}\left(\frac{\partial x^i}{\partial \tilde{x}^j}\right)\dot{\tilde{x}}^k + \frac{\partial}{\partial t}\frac{\partial x^i}{\partial \tilde{x}^j} = \frac{d}{dt}\frac{\partial x^i}{\partial \tilde{x}^j}.$$

We are now in a position to prove covariance. We have

$$\begin{aligned}
\tilde{\alpha}_i &= \frac{\partial \mathcal{L}}{\partial \tilde{x}^i} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{\tilde{x}}^i} \\
&= \frac{\partial \mathcal{L}}{\partial x^j}\frac{\partial x^j}{\partial \tilde{x}^i} + \frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{\partial \dot{x}^j}{\partial \tilde{x}^i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{\partial \dot{x}^j}{\partial \dot{\tilde{x}}^i}\right) \\
&= \frac{\partial \mathcal{L}}{\partial x^j}\frac{\partial x^j}{\partial \tilde{x}^i} + \frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{d}{dt}\frac{\partial x^j}{\partial \tilde{x}^i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}^j}\frac{\partial x^j}{\partial \tilde{x}^i}\right) \\
&= \frac{\partial x^j}{\partial \tilde{x}^i}\left(\frac{\partial \mathcal{L}}{\partial x^j} - \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{x}^j}\right),
\end{aligned}$$

exactly as we sought to show.

The immediate advantage that comes from this result is a freedom to solve the Euler-Lagrange equations in whatever coordinates we choose. It is easy to see that if a covariant vector vanishes in one coordinate system, it vanishes in any coordinate system, so the Euler-Lagrange equations of motion are equivalent in all coordinates.

Example 1.1. A particle is constrained to move on the surface $z = -\frac{R^2}{\sqrt{x^2+y^2}}$, where $R = \text{const.}$ A gravitational field provides a force $\boldsymbol{F} = -mg\hat{\boldsymbol{z}}$. Determine the equations of motion, and determine the angular velocity at which the particle must rotate to maintain a stable orbit at some fixed value of $r = \sqrt{x^2+y^2}$.

Solution: The particle has only two degrees of freedom. We will use polar coordinates in the xy-plane. Using $x = r\cos\theta$, $y = r\sin\theta$, and $z = -R^2/r$, we have

$$\begin{aligned}
T &= \frac{m}{2}\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) \\
&= \frac{m}{2}\left((1 + (R/r)^4)\dot{r}^2 + r^2\dot{\theta}^2\right).
\end{aligned}$$

The potential is $V = mgz = -\frac{mgR^2}{r}$. Therefore, the Lagrangian is

$$\mathcal{L} = \frac{m}{2}\left((1 + r^{-4})\dot{r}^2 + r^2\dot{\theta}^2\right) + \frac{mgR^2}{r}.$$

The equations of motion are

$$\begin{aligned}
\frac{d}{dt}\left(m(1 + (R/r)^4)\dot{r}\right) &= -2mR^4 r^{-5}\dot{r}^2 + mr\dot{\theta}^2 - \frac{mgR^2}{r^2}, \\
\frac{d}{dt}\left(mr^2\dot{\theta}\right) &= 0.
\end{aligned}$$

We recognize the second equation as the conservation of angular momentum.

In order to have a stable orbit, $\dot{r} = 0$, and the first equation of motion gives

$$0 = mr\dot{\theta}^2 - \frac{mgR^2}{r^2}.$$

This means the angular velocity is $\dot{\theta} = \sqrt{\frac{gR^2}{r^3}}$.

1.2 Cyclic Variables and Noether's Theorem

The form of the Euler-Lagrange equations invites a simple physical interpretation in some circumstances. If the Lagrangian is independent of some coordinate q, we call q a *cyclic coordinate*. The Euler-Lagrange equation of a cyclic coordinate q is

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}}\right) = \frac{\partial \mathcal{L}}{\partial q} = 0.$$

Therefore, the quantity $\frac{\partial \mathcal{L}}{\partial \dot{q}}$ is conserved. We define $p_q \equiv \frac{\partial \mathcal{L}}{\partial \dot{q}}$ to be the generalized momentum of the coordinate q. Then this result can be stated in a simple way:

Theorem 1.1. If q is a cyclic coordinate, p_q is a constant of motion.

The proof is as above. For instance, in Example 1.1, the Lagrangian was independent of θ, so θ was a cyclic coordinate. This implied conservation of p_θ, which is better known as angular momentum.

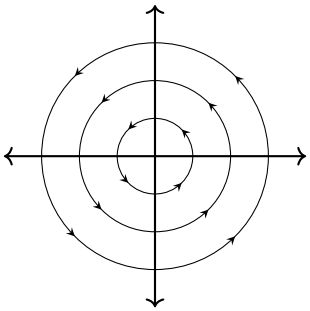
This is a useful fact, but it depends on choosing the right coordinates for the Lagrangian. If we had instead written the Lagrangian in Example 1.1 in terms of Cartesian coordinates x and y, there would have been no cyclic coordinates and we would not have discovered the conserved angular momentum.

The crucial fact, whether or not we write the Lagrangian using the coordinate θ, is that there is a rotational symmetry in the problem. This is the reason that θ is a cyclic coordinate, should it be used. Ideally, we would like to be able to detect the conserved quantity, angular momentum, from the symmetry alone. This will lead us to Noether's theorem.

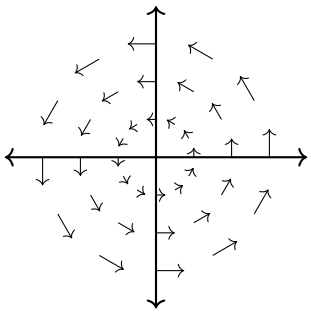
We must first be clear about what we mean by a symmetry in the Lagrangian. A rotation about the z axis carries each point through a trajectory, but these trajectories are related: as the rotation progresses, a given point in space will always flow in the same direction. This flow can be represented by a vector field, giving the derivative of the trajectory with respect to the rotation parameter at each point. Figure 1 shows the relation between the trajectories and the vector field generating them.

Now, assume we have a vector field $\delta x^i(x)$ which generates a symmetry of the Lagrangian. This means that, if we solve the differential equation

$$\frac{dx^i}{d\xi} = \delta x^i(x)$$



(a) The trajectories of a rotation about the z axis.



(b) The vector field generating rotation about the z axis.

Figure 1

for the trajectory $x^i(\xi)$, then $L(x^i(\xi)) = L(x^i(0))$ for all ξ and all initial conditions $x^i(0)$. We can then make a crucial observation: if ξ itself were taken as a coordinate, it would be a cyclic coordinate. It follows that p_ξ is conserved.

We have formally solved the problem, but in order to determine p_ξ, we would need to construct a coordinate transformation which makes ξ into one of the coordinates and then find its momentum. This is a tedious process. We will make use of the covariance of the Euler-Lagrange vector, and the resulting coordinate freedom, to do better. If we were to transform to coordinates where $x_1 = \xi$, then the vector field of the symmetry would become the constant $\delta x^i = (1, 0, \ldots, 0)$. It follows that $p_\xi = p_i \delta x^i$. Since both quantities on the right are vectors, their contraction is an invariant scalar, and it is equal in all coordinate systems. In particular, it does not change if we use p_i and δx^i in the original coordinates. This removes any need for actually shifting to the second coordinate system. This result is Noether's theorem.

Theorem 1.2 (Noether's Theorem)**.** Let δx^i be a vector field generating a symmetry of the Lagrangian. Then $p_i \delta x^i$, where p_i is the vector of momenta, is a constant of motion called the Noether charge of the symmetry.

Example 1.2. Given the Lagrangian

$$\mathcal{L} = \frac{m}{2} \sum \dot{x}_i^2 - V(x_i x^i),$$

determine three constants of motion associated with rotation.

Solution: The potential depends only on $r^2 = x_i x^i$, so a rotation about any axis is a symmetry of the Lagrangian. The corresponding vector fields are

$$\begin{aligned} \delta_x^{(1)} &= (0, -x_3, x_2), \\ \delta_x^{(2)} &= (x_3, 0, -x_1), \\ \delta_x^{(3)} &= (-x_2, x_1, 0). \end{aligned}$$

It then follows immediately that the three conserved quantities are

$$L_1 = x_2 p_3 - x_3 p_2,$$
$$L_2 = x_2 p_1 - x_1 p_3,$$
$$L_3 = x_1 p_2 - x_2 p_1.$$

These are the components of a vector $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$, the angular momentum.

There is a slight generalization of cyclic variables, and a corresponding generalization of Noether's theorem, which will be very useful to us. If the Lagrangian is not independent of q, but the partial derivative takes the special form

$$\frac{\partial \mathcal{L}}{\partial q} = \frac{dA}{dt}$$

for some function A, then the Euler-Lagrange equations become

$$\frac{d}{dt}\left(p_q - A\right) = 0,$$

implying conservation of $p_q - A$. This can be understood as a symmetry of the action; since $S = \int \mathcal{L}\, dt$, changing $\mathcal{L}$ by a total time derivative only changes the action by a constant, which does not affect the equations of motion. Following our previous argument for Noether's theorem, we obtain the more general version:

Theorem 1.3 (Noether's Theorem)**.** Let δx^i be a vector field generating a symmetry of the action, via

$$\left.\frac{\partial \mathcal{L}(x^i(\xi))}{\partial \xi}\right|_{\xi=0} = \frac{dA}{dt}.$$

Then $p_i \delta x^i - A$, where p_i is the vector of momenta, is a constant of motion called the Noether charge of the symmetry.

Example 1.3. Consider a system of N particles interacting only among themselves through a pairwise potential $V(\Delta x_i)$. Show that their center of mass moves at a constant velocity.

Solution: The Lagrangian can be written as

$$\mathcal{L} = \frac{1}{2}\sum_{\alpha=1}^{N} m_i (\dot{x}_\alpha^i)^2 - \sum_{\alpha<\beta} V_{ij}(x_\alpha - x_\beta).$$

Consider the Galilean symmetry $x_\alpha^i \to x_\alpha^i - v^i t$. The parameter is the velocity boost v^i. Substi-

tuting into the Lagrangian and differentiating, we have

$$\begin{aligned}\left.\frac{\partial \mathcal{L}}{\partial v^i}\right|_{v^i=0} &= \frac{\partial}{\partial v^i}\left(\frac{1}{2}\sum_{\alpha=1}^{N} m_i(\dot{x}_\alpha^i - v^i)^2 - \sum_{\alpha<\beta} V_{ij}(x_\alpha - x_\beta)\right)_{v^i=0} \\ &= \sum_{\alpha=1}^{N} m_\alpha(-\dot{x}_{i,\alpha}) \\ &= -\frac{d}{dt}\left(\sum_{\alpha=1}^{N} m_\alpha x_{i,\alpha}\right).\end{aligned}$$

We therefore have a symmetry of the action. The generators, one for each direction of velocity, are

$$\delta x_j^i = -t\delta_j^i,$$

so Noether's theorem tells us that

$$-p_i t\,\delta x_j^i + \sum_{\alpha=1}^{N} m_\alpha x_{j,\alpha} = -p_j t + \sum_{\alpha=1}^{N} m_\alpha x_{j,\alpha}$$

is conserved. The second term is MX_j, where M is the total mass and X_j is the center of mass position. Thus, conservation of this quantity implies

$$\frac{d}{dt}(MX_j - p_j t) = M\dot{X}_j - p_j = 0,$$

so the center of mass moves with constant velocity $\frac{p_j}{M}$.

1.3 Hamiltonian Mechanics

The machinery of Noether's theorem allows us, in particular, to derive the conservation of energy. We will use time translation symmetry, which is very subtle. The vector field is

$$\delta x^i = \dot{x}^i,$$

and so the integrated trajectories are simply $x^i(t)$, the physical trajectories. It follows that

$$\frac{\partial \mathcal{L}(x^i(t))}{\partial t} = \frac{\partial \mathcal{L}}{\partial x^i}\dot{x}^i + \frac{\partial \mathcal{L}}{\partial \dot{x}^i}\ddot{x}^i = \frac{d\mathcal{L}}{dt}.$$

Note that the last equality relies on the assumption that $\frac{\partial \mathcal{L}}{\partial t} = 0$. If there is explicit time-dependence in the Lagrangian, energy need not be conserved.

Since the Lagrangian is changing by a total time derivative, we can apply Noether's thoerem. We obtain the conserved quantity

$$\mathcal{H} = p_i\dot{x}^i - \mathcal{L}.$$

This is called the *Hamiltonian*, and it coincides with the energy. Indeed, for $\mathcal{L} = T - V$, we find

$$\mathcal{H} = \frac{\partial L}{\partial \dot{x}^i}\dot{x}^i - (T - V) = 2T - (T - V) = T + V,$$

the total energy.

The Hamiltonian is written as a function of coordinates and their momenta, unlike the Lagrangian which was written as a function of coordinates and their derivatives. We therefore must invert the relation between $\dot{x}_i$ and p_i to write $\dot{x}^i(p)$, such that

$$\mathcal{H} = p_i\dot{x}^i(p) - \mathcal{L}(x^i, \dot{x}^i(p_i)).$$

Using this expression, we can find the derivatives of the Hamiltonian. They are

$$\begin{aligned}\frac{\partial \mathcal{H}}{\partial x^i} &= -\frac{\partial \mathcal{L}}{\partial x^i} = -\dot{p}_i, \\ \frac{\partial \mathcal{H}}{\partial p^i} &= \dot{x}^i + p^j\partial_{p_j}\dot{x}^i - \partial_{p_j}\dot{x}^i\partial_{\dot{x}_j}\mathcal{L} = \dot{x}^i,\end{aligned}$$

where in the second equation we used the fact that $p^j = \partial_{\dot{x}_j}\mathcal{L}$. We see that the Hamiltonian generates first-order equations of motion for the positions and momenta:

$$\dot{x}^i = \frac{\partial \mathcal{H}}{\partial p_i}, \qquad \dot{p}^i = -\frac{\partial \mathcal{H}}{\partial x_i}.$$

These are known as the canonical equations of motion.

Mathematical aside: The elegant form of the canonical equations of motion is not an accident. They arise in this way because the Hamiltonian is the *Legendre transform* of the Lagrangian. The Legendre transform of a convex function $F(x^i)$ is defined to be

$$F^*(y^i) = \sup_{x^i}(y_i x^i - F(x^i)).$$

With suitable growth conditions on F, the supremum for $F^*(y^i)$ is achieved at some x^i. This implies

$$\frac{\partial}{\partial x^i}(y_i x^i - F(x^i)) = y_i - \frac{\partial F}{\partial x^i} = 0,$$

so in fact $y_i = \frac{\partial F}{\partial x^i}$. Appealing to the convexity of F, we can invert this relation to find x^i as a function of y, and so we have

$$F^*(y^i) = y_i x^i(y) - F(x^i(y)).$$

The Legendre transform is an involution, meaning $F^{**} = F$. We prove this in two steps. First, from the definition of F^*, it follows that

$$F^*(y^i) \geq y_i x^i - F(x^i) \implies F(x^i) \geq y_i x^i - F^*(y_i).$$

The inequality still holds if we take the supremum over the y^i on the right, so

$$F(x^i) \geq \sup_{y^i}(y_i x^i - F^*(y^i)) = F^{**}(x^i).$$

Conversely, we have

$$F^{**}(x^i) = \sup_{y^i}(y_i x^i - F^*(y^i)) = \sup_{y^i}\inf_{z^i}(y_i(x^i - z^i) + F(z^i)).$$

The right hand side is greater than or equal to its value for any particular choice of y^i, so we choose $y^i = \frac{\partial F}{\partial x_i}$. We then have

$$F^{**}(x^i) \geq \inf_{z^i}\left(\frac{\partial F}{\partial x_i}(x^i - z^i) + F(z^i)\right) = F(x^i),$$

where the last equality is due to the convexity of F.

Using this duality, it is easy to see that we have both

$$y_i = \frac{\partial F}{\partial x^i}, \qquad x_i = \frac{\partial F^*}{\partial y^i}.$$

We can now specialize to $F = \mathcal{L}(x^i, \dot{x}^i)$. We will ignore the dependence on x^i for the purpose of the Legendre transform. Indeed, the transform as we have developed it applies only to $\mathcal{L}(\dot{x}^i)$, as only this part of the Lagrangian is guaranteed to be convex (since kinetic energy is a positive definite quadratic form in velocity). The conjugate variables are $p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i}$, and the Legendre transform is $\mathcal{L}^* = \mathcal{H}(x^i, p^i)$. By duality, $\dot{x}^i = \frac{\partial \mathcal{H}}{\partial p_i}$, the first set of canonical equations of motion. The second set follows from the Euler-Lagrange equations.

The canonical equations of motion give all the time derivatives for a system in terms of the Hamiltonian. We can use this to build a powerful tool. Let $A(x^i, p^i, t)$ be some function. Then its total time derivative is

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \sum_i \frac{\partial A}{\partial x^i}\frac{dx^i}{dt} + \sum_i \frac{\partial A}{\partial p^i}\frac{dp^i}{dt}.$$

Using the canonical equations, we can rewrite this as

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + \sum_i \left(\frac{\partial A}{\partial x^i}\frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial A}{\partial p^i}\frac{\partial \mathcal{H}}{\partial x_i}\right).$$

The second term on the right no longer contains any time derivatives. We define it as the *Poisson bracket*. More generally, the Poisson bracket of two functions A and B is

$$(A, B) \equiv \sum_i \left(\frac{\partial A}{\partial x^i}\frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p^i}\frac{\partial B}{\partial x_i}\right).$$

Using this notation, we can write

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} + (A, \mathcal{H}).$$

In the common case where A has no explicit time dependence, the Hamiltonian generates the complete time dependence of A through the Poisson bracket.

It is striking that the Hamiltonian, which is the Noether charge of time translation symmetry, is generating time derivatives. In fact, this holds more generally. For example, p_1 is the conserved quantity arising from translational symmetry in the x^1 direction, and

$$(A, p_1) = \sum_i \left(\frac{\partial A}{\partial x^i}\frac{\partial p_1}{\partial p_i} - \frac{\partial A}{\partial p^i}\frac{\partial p_1}{\partial x_i}\right) = \frac{\partial A}{\partial x^1}.$$

Note that this implies

$$(x_i, p_j) = \delta_{ij},$$

where δ_{ij} is the Kronecker symbol (equal to 1 when $i = j$, and 0 otherwise). This fact can be very useful when computing Poisson brackets.

We can prove that the relationship between constants of motion and their symmetries holds generally. Let Q be a constant of motion; this means that

$$(Q, H) + \frac{\partial Q}{\partial t} = 0.$$

Note that we will not assume $\frac{dQ}{dt} = 0$, since this holds only when the equations of motion are satisfied, but we are seeking an identity which holds even for symmetry transformations which violate the equations of motion. In order to apply Noether's theorem, we will need to express the Lagrangian in terms of the Hamiltonian. Rearranging the definition of the Hamiltonian gives

$$\mathcal{L} = p_i \dot{x}^i - \mathcal{H}.$$

The variables of this Lagrangian can be taken to be coordinates $\zeta^I = (x^i, p^i)$ (where capital indices are in the range $1, \ldots, 2n$, with $1, \ldots, n$ indexing position and $n+1, \ldots, 2n$ indexing momentum), and their derivatives $\dot{\zeta}^I = (\dot{x}^i, \dot{p}^i)$. Now, consider the generator of a (possible) symmetry,

$$\delta\zeta^I = (\zeta^I, Q) = \begin{cases} \frac{\partial Q}{\partial p_i} & 1 \le I \le n, \\ -\frac{\partial Q}{\partial x_i} & n < I \le 2n \end{cases}.$$

If we solve the differential equations $\frac{d\zeta^I}{d\xi} = \delta z^I$ for $\zeta^I(\xi)$, we find

$$\begin{aligned} \left.\frac{d\mathcal{L}(\zeta^I(\xi))}{d\xi}\right|_{\xi=0} &= \delta p^i \dot{x}_i + p_i \delta\dot{x}^i - \frac{d\mathcal{H}(\zeta^I(\xi))}{d\xi} \\ &= \delta p^i \dot{x}_i + p_i \delta\dot{x}^i - \frac{\partial \mathcal{H}}{\partial x^i}\delta x^i - \frac{\partial \mathcal{H}}{\partial p^i}\delta p^i. \end{aligned}$$

We do not have an expression for $\delta\dot{x}^i$, but we can get around this difficulty by writing

$$p_i \delta\dot{x}^i = \frac{d}{dt}\left(p_i \delta x^i\right) - \dot{p}_i \delta x^i.$$

We can then substitute the assumed values of $\delta\zeta^I = (\delta x^i, \delta p^i)$, and find

$$\begin{aligned} \left.\frac{d\mathcal{L}(\zeta^I(\xi))}{d\xi}\right|_{\xi=0} &= -\frac{\partial Q}{\partial x_i}\dot{x}_i - \dot{p}_i \frac{\partial Q}{\partial p_i} + \frac{d}{dt}\left(p_i \delta x^i\right) - \frac{\partial \mathcal{H}}{\partial x^i}\frac{\partial Q}{\partial p_i} + \frac{\partial \mathcal{H}}{\partial p^i}\frac{\partial Q}{\partial x_i}. \\ &= -\left(\frac{dQ}{dt} - \frac{\partial Q}{\partial t}\right) + \frac{d}{dt}\left(p_i \delta x^i\right) + (Q, \mathcal{H}) \\ &= \frac{d}{dt}\left(p_i \delta x^i - Q\right), \end{aligned}$$

where in the last line we have used the fact that Q is a constant of motion. Since the Lagrangian is changing only by a total time derivative, the transformation $\delta\zeta^I$ is indeed a symmetry of the action. According to Noether's theorem, it generates a conserved charge

$$p_i \delta x^i - \left(p_i \delta x^i - Q\right) = Q.$$

This result is summarized in the following theorem.

Theorem 1.4. A constant of motion generates a symmetry through its Poisson bracket. The Noether charge of this symmetry is the constant of motion which generates it.

Example 1.4. Determine the Poisson brackets (L_i, L_j), where L_i is the angular momentum and $i, j = 1, 2, 3$. Interpret your answer in terms of Theorem 1.4.

Solution: The brackets with $i = j$ are clearly zero, and $(L_i, L_j) = -(L_j, L_i)$, so we have only three quantities to compute, (L_1, L_2), (L_2, L_3), and (L_3, L_1). Since the labeling of axes is arbitrary, all these are in fact equal. We may then compute one explicitly:

$$\begin{aligned}(L_1, L_2) &= (x_2p_3 - x_3p_2, x_3p_1 - x_1p_3)\\ &= (x_2p_3, x_3p_1) + (x_3p_2, x_1p_3) - (x_3p_2, x_3p_1) - (x_2p_3, x_1p_3)\\ &= x_2p_1(p_3, x_3) + x_1p_2(x_3, p_3)\\ &= x_1p_2 - x_2p_1\\ &= L_3.\end{aligned}$$

Note that the crucial fact used here was $(x_i, p_j) = \delta_{ij}$.

To interpret this fact, we recall that the components of angular momentum are the Noether charges of rotational symmetry. Thus,

$$(L_1, L_2) = \frac{\partial L_1}{\partial \theta_2},$$

where θ_2 is the angle about the x_2 axis. Rotating the angular momentum in the x_1x_3 plane moves L_1 in the direction of L_3, which accounts for our result.

The Poisson brackets of angular momentum can all be expressed in a compact way by

$$(L_i, L_j) = \epsilon_{ijk}L^k.$$

The symbol ϵ_{ijk} is called the *Levi-Civita symbol.* It is equal to 1 when ijk is a cyclic permutation of 123, -1 when ijk is a non-cyclic permutation of 123, and 0 otherwise.

2 Group Theory

The entirety of this section might be considered a mathematical aside. The remainder of the notes can be understood fairly well without any detailed knowledge of group theory. However, this background (especially regarding Lie groups and their algebras) will make later constructions feel more natural, and so reading this section is encouraged.

2.1 Groups and Homomorphisms

A *group* is one of the simplest algebraic structures. A group G consists of a set, which we will denote UG, and an operation $\circ$ satisfying the following properties:

- Associativity: $a \circ (b \circ c) = (a \circ b) \circ c$ for all $a, b, c \in UG$
- Identity: there exists $e \in G$ such that, for all $a \in G$, $e \circ a = a \circ e = a$
- Inverse: for all $a \in G$, there exists $a^{-1} \in G$ such that $a \circ a^{-1} = a^{-1} \circ a = e$

If additionally the operation is commutative, satisfying $a \circ b = b \circ a$ for all $a, b \in UG$, we call G an *Abelian group*. From now on we will ignore the distinction between G and UG, and say $g \in G$ when in fact $g \in UG$. Additionally, we suppress the operation $\circ$, and write ab for $a \circ b$.

For example, consider the following group, known as the Klein four group V_4. It can be presented as a table specifying the operation for each pair of elements:

	e	a	b	ab
e	e	a	b	ab
a	a	e	ab	b
b	b	ab	e	a
ab	ab	b	a	e

We can also specify the group in terms of generators (a and b) and their relations, as $V_4 = \langle a, b \mid a^2 = b^2 = (ab)^2 = e \rangle$. Note that the information given here is sufficient to construct the multiplication table above.

Groups are useful to us because the symmetries of an object (mathematical or physical) always form a group under composition. Associativity is clear for the composition operation, there is an identity operation (do nothing), and every symmetry can be "undone," giving its inverse.

For example, consider a square in the plane. It can be transformed into itself by rotations of 0, $\pi/2$, π, and $3\pi/2$, or by reflections through any of four lines of symmetry. This group is called D_4, the dihedral group on four elements. In general, D_n is the symmetry group of an n-gon.

Example 2.1. What is the symmetry group D_n of a regular n-gon in the plane? Enumerate its elements and then give a presentation of the group structure.

Solution: As a starting example, consider a square. It can be transformed into itself by rotations of 0, $\pi/2$, π, and $3\pi/2$, or by reflections through any of four lines of symmetry.

In general, we will have n rotations and n reflections, for a total of $2n$ elements. These can all be generated by a single rotation r and a single reflection s. The rotations are $e, r, r^2, \ldots, r^{n-1}$, and the reflections are $s, rs, r^2s, \ldots, r^{n-1}s$. The way rotations and reflections interact among themselves is specified by the conditions $r^n = e$ and $s^2 = e$. The full group structure is born out when we specify in addition that rs is also a reflection, so $(rs)^2 = e$. The group presentation is

$$D_n = \langle r, s \mid r^n = s^2 = (rs)^2 = e \rangle.$$

We can define a special kind of function over a group called a *homomorphism*. In abstract algebra broadly, a homomorphism is a map which respects the structure of its domain. For groups, this means a homomorphism $\phi : G \to H$ is a function satisfying

$$\phi(g_1 \circ g_2) = \phi(g_1) \circ \phi(g_2) \quad \forall g_1, g_2 \in G.$$

Note that the operation $\circ$ on the left hand side takes place in G, while the $\circ$ on the right takes place in H. If we have homomorphisms $\phi : G \to H$ and $\psi : H \to G$, such that $\phi\psi = 1_H$ (the identity on H) and $\psi\phi = 1_G$ (the identity on G), we call this an *isomorphism*.

Example 2.2. Consider the groups $(\mathbb{R}, +)$, the real numbers under addition, and $(\mathbb{R}^+, \times)$, the positive real numbers under multiplication. Construct an isomorphism between the two groups.

Solution: Consider the maps $\phi : (\mathbb{R}, +) \to (\mathbb{R}^+, \times)$ and $\psi : (\mathbb{R}^+, \times) \to (\mathbb{R}, +)$ defined by

$$\phi(x) = e^x, \qquad \psi(x) = \log x.$$

These are homomorphisms, since

$$\begin{aligned} \phi(x + y) &= e^{x+y} = e^x e^y = \phi(x) \times \phi(y), \\ \psi(xy) &= \log(xy) = \log(x) + \log(y) = \psi(x) + \psi(y). \end{aligned}$$

Additionally, they are inverses. Thus, this pair forms an isomorphism.

If we have a homomorphism $\phi : H \to G$ which is *injective*, such that $\phi(h_1) = \phi(h_2)$ implies $h_1 = h_2$, we say H is a *subgroup* of G. The notation is $H \subset G$. The homomorphism identifies each element of H with a distinct element of G, and thereby embeds the group structure of H into that of G, which justifies the name. For example, V_4 is a subgroup of D_4, via the homomorphism defined by $\phi(a) = r^2$ and $\phi(b) = s$. If $H \subset G$ through ϕ, we write $g \in H$ as an abbreviation for $g \in \operatorname{im} \phi$.

Whenever we have $H \subset G$, we can use H to define a relation $\sim_H^l$ on H. We say $g_1 \sim_H^l g_2$ whenever g_1 is "a left H-move" away from g_2; that is, for some $h \in H$, $g_1 = hg_2$. We can express this condition as $g_1 g_2^{-1} \in H$. We can prove three properties of this relation:

- Reflexivity: $g \sim_H^l g$, since $gg^{-1} = e \in H$
- Symmetry: $g_1 \sim_H^l g_2 \implies g_2 \sim_H^l g_1$, since if $g_1 g_2^{-1} \in H$, then so is $(g_1 g_2^{-1})^{-1} = g_2 g_1^{-1}$
- Transitivity: if $g_1 \sim_H^l g_2$ and $g_2 \sim_H^l g_3$, then $g_1 \sim_H^l g_3$, since if $g_1 g_2^{-1} \in G$ and $g_2 g_3^{-1} \in G$, then so is $(g_1 g_2^{-1})(g_2 g_3^{-1}) = g_1 g_3^{-1}$

These three properties show that $\sim_H^l$ is an equivalence relation. An equivalence relation on a set partitions the set into equivalence classes. The equivalence classes of $\sim_H^l$ are called the left cosets of H.

Every left coset is of the form

$$Hg = \{hg \mid h \in H\}.$$

It is simple to verify that every element of this set is equivalent under $\sim_H^l$, and also that this set contains every element equivalent to g. It is also clear that the cardinality of this set is equal to the cardinality of H. The number of these cosets is denoted $[G : H]$. For finite groups, it follows that

$$|G| = [G : H] \cdot |H|.$$

This implies in particular that $|H|$ is a divisor of $|G|$. This fact is known as *Lagrange's theorem.*

Everything we have developed for left cosets holds also for right cosets. We can define an equivalence relation $\sim_H^r$ by $g_1 \sim_H^r g_2$ whenever $g_1^{-1} g_2 \in H$. Its equivalence classes are right cosets gH. Crucially, the right cosets need not be the same as the left cosets; they may form an entirely different partition of G.

If, however, the left and right cosets are identical, then the cosets themselves take on structure. When this is the case, we say that H is a normal subgroup of G, and write $H \lhd G$. Consider two left cosets, Hg_1 and Hg_2. Generic elements of these cosets are $h_1 g_1$ and $h_2 g_2$, and their product is $h_1 g_1 h_2 g_2$. Since we are assuming left and right cosets to be identical, $g_1 h_2 \in g_1 H = Hg_1$, so $g_1 h_2 = h g_1$ for some $h \in H$. It follows that $h_1 g_1 h_2 g_2 = h_1 h g_1 g_2 \in H g_1 g_2$. Moreover, it is simple to show that every element of $Hg_1 g_2$ can be formed as a product in this way. Therefore, we have an equality of sets

$$(Hg_1)(Hg_2) = Hg_1 g_2,$$

where the left hand side is taken to mean all possible products formed from members of the two cosets.

In this way, the cosets can inherit the structure of G, modulo equivalence under H. In fact, under this product operation, the cosets themselves form a group: the identity is H itself, and the inverse of Hg is Hg^{-1}. The group of cosets is called the factor group of G by H, and denoted G/H. The cardinality of the factor group is $|G/H| = [G : H]$. There is a homomorphism $\pi : G \to G/H$, defined by $\pi(g) = Hg$, which is called the canonical projection.

Example 2.3. Determine the factor group $\mathbb{Z}/n\mathbb{Z}$ and the canonical projection mapping associated with it.

Solution: First, we note that $n\mathbb{Z} = \{\ldots, -2n, -n, 0, n, 2n, \ldots\}$ is indeed a subgroup of $\mathbb{Z}$ (where the operation is addition). We must also verify that $n\mathbb{Z}$ is a normal subgroup of $\mathbb{Z}$. However, since $\mathbb{Z}$ is Abelian, all subgroups are normal, since $gH = Hg$ trivially.

Two elements $a, b \in \mathbb{Z}$ are in the same coset of $n\mathbb{Z}$ whenever there exists $c \in n\mathbb{Z}$ such that $a = b + c$. Writing $c = nd$, where $d \in \mathbb{Z}$, we have $a = b + nd$. This is equivalent to $a \equiv b \pmod{n}$. Thus, the cosets of $n\mathbb{Z}$ in $\mathbb{Z}$ are sets of numbers which are congruent modulo n. There are n of these cosets, corresponding to representative elements $\{0, \ldots, n-1\}$.

The group $\mathbb{Z}/n\mathbb{Z}$ is the group of these cosets under the inherited operation from $\mathbb{Z}$. If we label cosets by their representative elements, then adding cosets corresponds to adding representative elements, and then possibly substracting a multiple of n to return to a representative element in $\{0, \ldots, n-1\}$. This procedure describes addition modulo n. Thus, $\mathbb{Z}/n\mathbb{Z}$ is simply the integers modulo n under addition. The projection mapping $\pi : \mathbb{Z} \to \mathbb{Z}/n\mathbb{Z}$ sends an integer to its coset, which can be labeled by its representative element; we think of π as "modding out" a number by n.

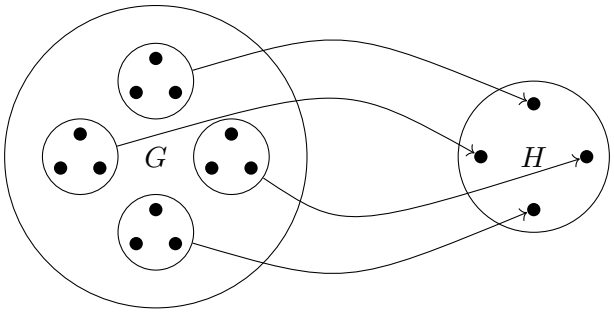


Figure 2: Each coset of $\ker\phi$ is sent by $\phi : G \to H$ to a distinct element of $\operatorname{im}\phi$.

Whenever $H \lhd G$, we can form G/H and the canonical projection $\pi : G \to G/H$, and then $H = \ker\pi$. Thus, every normal subgroup is the kernel of a homomorphism. The converse holds as well: if $\phi : G \to H$ is a homomorphism, then $\ker\phi$ is a normal subgroup of G. The proof that it is a subgroup is simple; to show it is a normal subgroup, we let $a \in \ker\phi$, and then $\phi(gag^{-1}) = \phi(g)\phi(a)\phi(g^{-1}) = \phi(g)\phi(g^{-1}) = e$, so $gag^{-1} \in \ker\phi$. It follows that $g(\ker\phi) = (\ker\phi)g$, so left and right cosets are equal, and $\ker\phi \lhd G$. When we form the factor group $G/\ker\phi$, we obtain $\operatorname{im}\phi$, as should be clear from Figure 2. This result is called the first isomorphism theorem.

Theorem 2.1 (First Isomorphism Theorem)**.** Let G be a group and $\phi : G \to H$ be a homomorphism. Then $\ker\phi \lhd G$, and

$$\frac{G}{\ker\phi} \simeq \operatorname{im}\phi.$$

In addition to taking subgroups and factor groups, we can form larger groups via the direct product. The direct product of groups G and H, denoted $G \times H$ is the set $\{(g,h) \mid g \in G, h \in H\}$ together with the operation $(g_1,h_1) \circ (g_2,h_2) = (g_1g_2, h_1h_2)$. The injective maps $\phi_G : G \to G \times H$ with $phi_G(g) = (g,e)$, and $\phi_H : H \to G \times H$ with $\phi_H(h) = (e,h)$, exhibit G and H respectively as subgroups of $G \times H$. Additionally, the projections $\pi_G : G \times H \to G$, with $\pi_G((g,h)) = g$, and $\pi_H : G \times H \to H$, with $\pi_H((g,h)) = h$, have kernels $\ker\pi_G = H$ and $\ker\pi_H = G$. Therefore, by Theorem 2.1, G and H are normal subgroups of $G \times H$ and

$$\frac{G \times H}{G} \simeq H, \qquad \frac{G \times H}{H} \simeq G.$$

It is tempting to conclude that the factor group and the direct product are inverses, in the sense that $G/H \simeq K$ exactly when $H \times K \simeq G$. However, this is not generally the case. For example, consider the group $\mathbb{Z}/4\mathbb{Z} = \{0,1,2,3\}$, and its subgroup $\{0,2\}$ isomorphic to $\mathbb{Z}/2\mathbb{Z}$. We have

$$\frac{\mathbb{Z}/4\mathbb{Z}}{\mathbb{Z}/2\mathbb{Z}} \simeq \mathbb{Z}/2\mathbb{Z},$$

but $(\mathbb{Z}/2\mathbb{Z}) \times (\mathbb{Z}/2\mathbb{Z}) \not\simeq \mathbb{Z}/4\mathbb{Z}$.

This distinction is often highlighted using exact sequences. An *exact sequence* is a sequence of groups and homomorphisms,

$$\cdots \longrightarrow G_{i-1} \xrightarrow{\phi_{i-1}} G_i \xrightarrow{\phi_i} G_{i+1} \longrightarrow \cdots,$$

such that $\operatorname{im}\phi_{i-1} = \ker\phi_i$. A *short* exact sequence is one of the form

$$0 \longrightarrow G \xrightarrow{\phi} K \xrightarrow{\psi} H \longrightarrow 0,$$

where $0 = \{e\}$ is the trivial group. The first (last) homomorphism is fixed because its domain (range) is the trivial group. The exactness criterion implies that $\ker\phi = 0$, so ϕ is injective and $G \subset K$, and $\operatorname{im}\psi = H$, so ψ is surjective. Additionally, $\ker\psi = \operatorname{im}\phi$, so by Theorem 2.1, $K/G \simeq H$. If in addition $K \simeq G \times H$, we call the sequence a *split* exact sequence.

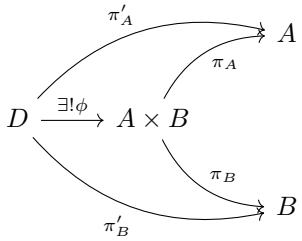
Mathematical aside: Many algebraic notions, including those of group theory, can be cast into a very elegant form by using the language of category theory.

A *category* is a collection of objects and morphisms between them, such that morphisms $\alpha : A \to B$ and $\beta : B \to C$ can be composed to give $\beta\alpha : A \to C$, and for each object there is an identity morphism $1_A : A \to A$ which composes in the expected way. We denote the set of morphisms from A to B by $\operatorname{Hom}(A, B)$.

This simple concept can easily capture a wide variety of structures. For example, a group is a category consisting of a single object where all morphisms are isomorphisms, i.e., for any $\alpha : A \to A$ there exists $\alpha^{-1} : A \to A$ such that $\alpha\alpha^{-1} = \alpha^{-1}\alpha = 1_A$. The morphisms represent the group elements. More typically, we form the category Grp consisting of all groups, with morphisms being the homomorphisms between them.

We say an object $A \in \mathsf{C}$ is *initial* if, for all $B \in \mathsf{C}$, $\operatorname{Hom}(A, B)$ is a singleton set. Likewise, $A \in \mathsf{C}$ is *terminal* if, for all $B \in \mathsf{C}$, $\operatorname{Hom}(B, A)$ is a singleton set. At this point it is worth noting that each category has an opposite, denoted C^{op}, which is identical to C except with all the morphisms reversed; since an initial object of C is a terminal object of C^{op}, we say these are dual concepts.

Constructions in a category can be specified using universal properties. An object is universal if it is initial or terminal in some suitably constructed category. As a prototypical example, the categorical product of two objects $A, B \in C$ is an object $A \times B$ together with projection maps π_A and π_B, such that any other object $D \in \mathsf{C}$ with projection maps factors in the following manner:



The above is a *commutative diagram*; it expresses the equality of all paths between two points in the diagram as morphisms. For example, in this case, $\pi'_A = \pi_A \circ \phi$ and $\pi'_B = \pi_B \circ \phi$. This shows that the product is in some sense the smallest group containing all the data of both of its factors.

2.2 Representations of Finite Groups

The set of all $n \times n$ invertible complex matrices, under matrix multiplication, forms a group. It is called $GL(n, \mathbb{C})$, the general linear group of n dimensions over $\mathbb{C}$. A homomorphism $\rho : g \to GL(n, \mathbb{C})$ is called an n-dimensional *representation* of G.

Every group has at least one representation, called the *trivial representation*. The trivial representation is one-dimensional, and the homomorphism $\rho : G \to GL(n, \mathbb{C})$ is $\rho(g) = 1$. This is obviously a homomorphism, but it does not preserve any information about the structure of G.

If a representation consists of an injective homomorphism, we call it a *faithful* representation. Every finite group has at least one faithful representation as well. We can form it using permutation matrices. First, note that for a fixed $g \in G$, the set $\{gg' \mid g' \in G\}$ contains each element of G exactly once, and so left multiplication by g induces a permutation of the group elements. Multiplication by gh then consists of composing the permuation induced by g with that induced by h. Now, let $n = |G|$, and consider the homomorphism $\rho_r : G \to GL(n, \mathbb{C})$ defined by

$$\rho_r(g)_{ij} = \begin{cases} 1 & \text{if } gg_i = g_j, \\ 0 & \text{otherwise} \end{cases}.$$

The indexing g_i of the group elements is arbitrary. For example, the regular representation of $\mathbb{Z}_3 \equiv \mathbb{Z}/3\mathbb{Z} = \{e, a, a^2\}$ is given by

$$\rho_r(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \rho_r(a) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \rho_r(a^2) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

You can verify for yourself that this is a homomorphism.

An n-dimensional representation of a group defines an *action* on the vector space $\mathbb{C}^n$. In general, an action is a homomorphism from a group to the group of transformations of some other object; in this case, the group of transformations of $\mathbb{C}^n$ is just $GL(n, \mathbb{C})$. The action of $g \in G$ on a vector $v \in \mathbb{C}^n$ is given by $g(v) = \rho(g) \cdot v$.

For any group action, we can define the *orbit* of an element x of the acted-upon set as

$$O(x) = \{gx \mid g \in G\}.$$

Every orbit forms an *invariant subset* under G, meaning that $\{gy \mid g \in G, y \in O(x)\} = O(x)$. We say an action is *transitive* on a set S if there are no nontrivial invariant subsets; that is, if $O(x) = S$ for all $x \in S$.

No representation of a finite group induces a transitive action. The reason for this is simple: since every $g \in G$ permutes the n elements of G, we must have $g^n = e$. Therefore, it is impossible to have $gv = \alpha v$ where $\alpha \in \mathbb{C}$ and $|\alpha| \neq 1$, because otherwise $g^n v = \alpha^n v \neq v$.

To make the ideas behind orbits and transitivity useful in the setting of representations, we extend all subsets to subspaces by linearity. Explicitly, we define the orbit space by

$$\overline{O}(x) = \operatorname{span} O(x) = \operatorname{span}\{gx \mid g \in G\}.$$

Each orbit space is an invariant subspace. In place of transitivity, we use the notion of irreducibility. A representation is irreducible if the action it induces has no nontrivial invariant subspaces. In this case, we call it an *irrep*, an abbreviation of irreducible representation.

Example 2.4. Determine whether the action of $\mathbb{Z}_3$ on $\mathbb{C}^3$ via ρ_r is irreducible. If it is reducible, determine its smallest invariant subspaces (the orbit spaces).

Solution: Consider the vector $\boldsymbol{v} = (1,1,1)$. It is left invariant by the action of each $g \in G$, so it is called a *fixed point*. Its orbit space is the one-dimensional span of $(1,1,1)$, so the representation is reducible.

Certainly $\text{span}\{(1,1,1)\}$ is one of the smallest invariant subspaces. Its orthogonal complement, the vectors (a,b,c) with $a+b+c=0$, is also an invariant subspace. Since this is two-dimensional, it may contain smaller invariant subspaces. The only smaller possibility is a one-dimensional invariant subspace, which must be (like $(1,1,1)$) a simultaneous eigenvector of $\rho_r(e)$, $\rho_r(a)$, and $\rho_r(a^2)$. Since $\rho_r(a^2) = \rho_r(a)^2$, these matrices do in fact have the same eigenvectors. They are

$$v_1 = (1,1,1), \qquad v_2 = (1,\omega^2,\omega), \qquad v_3 = (1,\omega,\omega^2),$$

where $\omega = e^{2\pi i/3}$. The spans of these vectors are all invariant subspaces.

A reducible representation can be reduced into irreps. To do this, we simply restrict the representation to each orbit space. For example, take the case of the regular representation of $\mathbb{Z}_3$. Its invariant subspaces, determined in Example 2.4, are

$$V_1 = \text{span}\{(1,1,1)\}, \qquad V_2 = \text{span}\{(1,\omega,\omega^2)\}, \qquad V_3 = \text{span}\{(1,\omega^2,\omega)\}.$$

For vectors in each of these subspaces, we can determine the restricted (one-dimensional) representations:

$$\begin{array}{llll} v \in V_1: & ev = v & av = v & a^2v = v \\ v \in V_2: & ev = v & av = \omega v & a^2v = \omega^2 v \\ v \in V_3: & ev = v & av = \omega^2 v & a^2v = \omega v. \end{array}$$

The crucial data here is the coefficients on the right hand side. Since $\mathbb{Z}_3$ acts on each invariant subspace differently, we have three distinct irreps. We say that the full representation is the *direct sum* (denoted $\oplus$) of these reduced components.

These are, in fact, all the irreps of $\mathbb{Z}_3$. This could be proved directly in the case of $\mathbb{Z}_3$ without great difficulty, but it is best understood as a consequence of an important and powerful theorem.

Theorem 2.2 (Grand Orthogonality Theorem)**.** Let $\rho_1 : G \to GL(m,\mathbb{C})$ and $\rho_2 : G \to GL(n,\mathbb{C})$ be irreps of G. If ρ_1 is equivalent to ρ_2, meaning $\rho_1(g) = U\rho_2(g)U^\dagger$ (where U is a unitary change-of-basis matrix independent of g), then

$$\sum_{g\in G} \rho_1(g)_{ij}\overline{\rho_2(g)_{ab}} = |G|\delta_{ia}\delta_{jb},$$

where δ is the Kronecker symbol. If ρ_1 and ρ_2 are inequivalent, then the same sum vanishes.

The proof of this can be found in any text on representation theory. It says that each component of the matrices in an irreducible representation forms one of an orthogonal set of vectors in $\mathbb{C}^{|G|}$. But such a set can have size no greater than $|G|$. An n-dimensional representation has n^2 components, so this means that if the inequivalent irreps have dimensions n_i, then $\sum n_i^2 \leq |G|$. This is enough to establish that there can be no more than three irreps of $\mathbb{Z}_3$. Another result of fundamental importance is that this inequality is always saturated:

$$\sum n_i^2 = |G|.$$

There is an additional result which constrains the number of representations of a group. It comes from considering the *character* of a representation. The character is a function on the group elements which gives the trace of their representation matrices. For example, the character χ_r of the regular representation ρ_r of $\mathbb{Z}_3$ is given by $\chi_r(e) = 3$, $\chi_r(a) = \chi_r(a^2) = 0$.

The characters of inequivalent representations are orthogonal in the sense of Theorem 2.2; indeed, this follows immediately from Theorem 2.2. However, treating the characters as vectors in $\mathbb{C}^{|G|}$ is often inefficient. For example, consider the group S_3 of permutations on three elements. It has a two-dimensional representation ρ, defined by

$$\rho(123) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\rho(231) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix} \qquad \rho(312) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\rho(213) = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix} \qquad \rho(321) = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & 1/2 \end{pmatrix} \qquad \rho(132) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

On each row, the matrices have the same trace. This is not a coincidence. We say two elements $g_1, g_2 \in G$ are *conjugate* if there exists h in G such that $g_1 = hg_2h^{-1}$. The conjugacy classes of a group are the sets of elements which are all conjugate to each other. This tends to partition a group in an intuitively comprehensible way. For example, in S_3 the conjugacy classes are identity (first row), 3-cycles (second row), and 2-cycles (or swaps, second row).

The fact that a character is the same for all elements of a conjugacy class is simple to prove. If $g_1 = hg_2h^{-1}$, then

$$\begin{aligned} \chi_\rho(g_1) &= \mathrm{tr}(\rho(g_1)) = \mathrm{tr}(\rho(hg_2h^{-1})) = \mathrm{tr}(\rho(h)\rho(g_2)\rho(h)^{-1}) \\ &= \mathrm{tr}(\rho(h)^{-1}\rho(h)\rho(g_2)) = \mathrm{tr}(\rho(g_2)) = \chi_\rho(g_2). \end{aligned}$$

Note that we have used the identity $\mathrm{tr}(ABC) = \mathrm{tr}(CAB)$.

In view of this, we should think of a character as a vector in $\mathbb{C}^{n_c}$, where n_c is the number of conjugacy classes of a group. We have

$$\sum_{g \in G} \chi_1(g)\overline{\chi_2(g)} = \sum_{i=1}^{n_c} k_i \chi_1(g_i)\overline{\chi_2(g_i)},$$

where g_i is a representative of the ith conjugacy class and k_i is the size of the ith conjugacy class. This defines an inner product over $\mathbb{C}^{n_c}$ (although not the Euclidean inner product, since we have

the weights k_i). There can be at most n_c orthogonal vectors in this space, so there can be at most n_c inequivalent irreps. In fact, this is always saturated: every finite group has as many representations as it has conjugacy classes.

In some cases, this fixes the number and dimensions of the irreps uniquely. For example, S_3 has six elements and three conjugacy classes, so we need three representations with dimensions n_i such that $n_1^2 + n_2^2 + n_3^2 = 6$. We must have $n_1 = n_2 = 1$ and $n_3 = 2$. The two-dimensional representation was given above, and has character $\chi_3 = (2, -1, 0)$ (where the components correspond to conjugacy classes of size 1, 2, and 3 respectively). One of the one-dimensional representations must be $\chi_1 = (1, 1, 1)$, the trivial representation. The remaining one is fixed by orthogonality; you can verify that $\chi_2 = (1, 1, -1)$ is orthogonal to χ_1 and χ_3 under the weighted inner product.

We now have sufficient information to form a character table S_3. A character table lists the characters of each irrep for each conjugacy class. We will label the one-dimensional representations A_1 and A_2, and the two-dimensional representation E_1. The table is below.

S_3	e [1]	(231) [2]	(213) [3]
A_1	1	1	1
A_2	1	1	-1
E_1	2	-1	0

Character tables can be used to decompose any representation into its irreps in a very simple way. If we have a reducible representation, then we can change the basis so that each basis vector belongs to an invariant subspace, and group the basis vectors according to their invariant subspace. The matrices of the representation then take a block diagonal form, where each block is a matrix of an irrep. It is then clear that the trace of the reducible representation matrix is the sum of the traces of its irrep components. This means the character of the representation is a sum of characters of irreps. Since the irrep characters form an orthogonal basis, we can decompose the character into its components in this basis, and thereby find the irreps which build the reducible representation.

Example 2.5. Decompose the regular representation of S_3 into irreps. Then give a general expression for the decomposition of a regular representation.

Solution: In the regular representation, only the identity element maps to a matrix with trace, and its trace is the size of the group. The character is thus $\chi = (6, 0, 0)$. Recalling from Theorem 2.2 that the irrep characters χ_i have norm $|G| = 6$, the coefficient of χ_i is $(\chi \cdot \chi_i)/(\chi_i \cdot \chi_i)$, where $\cdot$ is the inner product on characters. Computing these coefficients, we find that the regular representation decomposes as $A_1 \oplus A_2 \oplus 2E_1$.

In the general case, the character of the regular representation is $\chi = (|G|, 0, \ldots, 0)$. The identity is always in its own conjugacy class, and the character of the identity is the dimension of the representation. Thus, for an n_i-dimensional representation with character χ_i, we have $(\chi \cdot \chi_i)/(\chi_i \cdot \chi_i) = n_i$. It follows that the regular representation decomposes as

$$\rho_r = \bigoplus_i (\dim \rho_i)\rho_i,$$

where ρ_i are irreps.

Mathematical aside: In an Abelian group, every element forms its own conjugacy class, since $hgh^{-1} = hh^{-1}g = g$. We therefore have $n = |G|$ representations, with dimensions squared summing to n, so the only possibility is n one-dimensional representations. Since they are one-dimensional, the characters of the representations are equivalent to the representations themselves. We denote the set of characters (or irreps) of G by $\hat{G}$.

Recall that a representation $\chi \in \hat{G}$ is a homomorphism, so its defining property is $\chi(gh) = \chi(g)\chi(h)$. This is satisfied if we take $\chi(g) = \chi_1(g)\chi_2(g)$ where $\chi_1, \chi_2 \in \hat{G}$. Additionally, $\chi^{-1}(g) = (\chi(g))^{-1}$ satisfies the same condition. We can thus treat $\hat{G}$ as a group under multiplication of characters.

We can use the characters of an Abelian group to define the *Fourier transform*. Let $f : G \to \mathbb{C}$ be any complex-valued function on the group; its Fourier transform $\hat{f} : \hat{g} \to \mathbb{C}$ is defined to be

$$\hat{f}(\chi) = \sum_{g \in G} f(g)\overline{\chi(g)}.$$

The right hand side is simply the inner product we have already defined on for functions on groups. Since the characters in $\hat{G}$ form an orthogonal basis under this inner product, we can extract $f(g)$ from $\hat{f}$ via

$$\frac{1}{|G|}\sum_{\chi \in \hat{G}} \hat{f}(\chi)\chi(g) = \frac{1}{|G|}\sum_{\chi \in \hat{G}}\sum_{g' \in G} f(g')\overline{\chi(g')}\chi(g) = \frac{1}{|G|}\sum_{g' \in G} f(g')(|G|\delta_{gg'}) = f(g).$$

This defines the inverse Fourier transform. We can put this in a form more symmetric with the Fourier transform itself using a deep result, the Pontryagin duality theorem, which says that the double dual $\hat{\hat{G}}$ is isomorphic to G. Taking the Fourier transform of $\hat{f}$ and using Pontryagin duality, we have

$$f(g) = \hat{\hat{f}}(g) = \sum_{\chi \in \hat{G}} \hat{f}(\chi)g(\chi),$$

where $g(\chi) \equiv \hat{\hat{g}}(\chi) = \chi(g)$.

We can see the equivalence to the usual definition of the Fourier transform by looking at the characters of Abelian groups. For simplicity, we will restrict attention to $\mathbb{Z}_n$, $\mathbb{Z}$, and $\mathbb{R}$. The characters of $\mathbb{Z}_n$ are similar in form to the ones we derived for $\mathbb{Z}_3$. Expressing $\mathbb{Z}_n$ as $\langle a \mid a^n = e\rangle$, we can write the characters as $\chi_k(a^m) = e^{-2\pi ikm/n}$, where $k = 0, \ldots, n-1$. Then

$$\hat{f}(\chi_k) = \sum_{j=0}^{n-1} f(a^j)\chi_k(a^j) = \sum_{j=0}^{n-1} f(a^j)e^{-2\pi ikj/n}.$$

In the case of $\mathbb{Z}$, characters are $\chi_k(n) = e^{-2\pi ikn}$, for $k \in [0, 1)$. Thus, the Fourier transform of $f : \mathbb{Z} \to \mathbb{C}$ is

$$\hat{f}(\chi_k) = \sum_{n \in \mathbb{Z}} f(n)e^{-ikn}.$$

Finally, we consider the most common case, $\mathbb{R}$. The characters of $\mathbb{R}$ are $\chi_k(x) = e^{-2\pi ikx}$, for $k \in \mathbb{R}$. The Fourier transform of $f : \mathbb{R} \to \mathbb{C}$ is then

$$\hat{f}(\chi_k) = \int_{\mathbb{R}} f(x)e^{-2\pi ikx}\,dx.$$

Note that in each case, the Fourier transform could be considered as a function over the index. In the case of $\mathbb{R}$, the index also lives in $\mathbb{R}$. It is common to refer to the Fourier transform of $f : \mathbb{R} \to \mathbb{C}$ as another function $\hat{f} : \mathbb{R} \to \mathbb{C}$, even though formally it is a function on the dual group $\hat{\mathbb{R}}$.

2.3 Lie Groups and Lie Algebras

A Lie group is a group endowed with the structure of a differentiable manifold. The exact definition of a differentiable manifold is not essential for our purposes; a helpful example is a smooth surface. The group structure must be compatible with the manifold structure, in the sense that if h is near to k on the manifold, then gh is near to gk (that is, group multiplication is continuous).

A simple example of a Lie group is the group $SO(2)$ of rotations of a plane. The designation $SO(2)$ refers to special orthogonal 2×2 matrices, a subset of $GL(2, \mathbb{R})$. These matrices can be parametrized by a single angle θ as

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta. \end{pmatrix}$$

This suggests that the group manifold is a circle (also known as the sphere with one dimension, S^1), with θ being its coordinate. This is in fact the case. The action of $SO(2)$ on its manifold is simply rotation of the circle, which is clearly continuous.

We can choose to think of any point on the circle as the identity element e of the group. Once we have fixed e, all other points are fixed by the action of the group on itself, since we can set $ge = g$. More generally, each element of the group induces a *diffeomorphism* (a smooth invertible function) from the manifold onto itself, via its left action. This is exactly analogous to the idea of an element of a finite group inducing a permutation on the group elements. We define the left-translation operator $L_g : G \to G$ by $L_g h = gh$. There is a similar right-translation operator, $R_g h = hg$, but we will not be using it. Any point can be carried to any other point by a left-translation, via $L_{g'g^{-1}} g = g'$.

A diffeomorphism of a manifold induces a map on its vectors. Recall that a vector v on a manifold consists of components v^i which transform under a coordinate change as a type (1,0) tensor. That is, if we change from coordinates x^i to coordinates $\tilde{x}^i$, the vector components become

$$\tilde{v}^i = v^j \frac{\partial \tilde{x}^i}{\partial x^j}.$$

A diffeomorphism is not the same as a change of coordinates, since it moves points on the manifold. However, it is similar in the sense that a diffeomorphism $\phi : M \to N$ can be represented as a smooth function on the coordinates. Its Jacobian can also be used to find the change in vector components of a vector at p, via

$$\phi_* v^i = v^j \left. \frac{\partial \phi^i}{\partial x^j} \right|_p .$$

The operator ϕ_* is called the pushforward of ϕ.

Like any group, a Lie group can have subgroups. Of particular interest are subgroups of G which can be represented as homomorphisms $\phi : \mathbb{R} \to G$. Note that the subgroup need not be isomorphic to $\mathbb{R}$; generically, by Theorem 2.1, the subgroup will be isomorphic to $\mathbb{R}/\ker\phi$. These are called

one-parameter subgroups. They define a flow on the manifold. For example, consider $SO(3)$, the group of rotations of three-dimensional Euclidean space. A one-parameter subgroup is defined by the homomorphism

$$\phi(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The one-parameter subgroup contains rotations about the z axis, and it is in fact isomorphic to $SO(2)$.

These subgroups are of particular interest because together they can often tell us about the group as a whole, while individually they are much simpler than the full Lie group. This is so because, under some relatively weak assumptions, every element $g \in G$ can be reached by moving in some direction away from the identity, this direction defining a one-parameter subgroup. We will make this connection more clear in the following, and use it to find the Lie algebra of a Lie group.

The flow defined by a one-parameter subgroup can be represented equivalently by a vector field on the manifold. Let the one-parameter subgroup be $\phi^\mu(t)$, where μ is an index for the coordinates on the manifold. Then we have a vector field

$$X^\mu(\phi(t)) = \frac{d\phi^\mu(t)}{dt}.$$

Alternatively, we can think one of the one-parameter subgroup as the solution to this differential equation.

As written, X^μ is only defined on the subgroup $\operatorname{im}\phi$. There is a natural way to extend it to the entire group. We first note that X^μ as defined so far enjoys a compatibility property with the group, through the left-translation operator. To act on vectors, we need to use the pushforward of left-translation. Acting with such an operator, we have

$$L_{\phi(s)*}X^\mu(\phi(t)) = L_{\phi(s)*}\frac{d\phi^\mu(t)}{dt} = \frac{d\phi^\nu(t)}{dt}\left.\frac{\partial\phi^\mu(s)}{\partial x^\nu}\right|_{\phi(t)} = \frac{d\phi^\mu(t+s)}{dt} = X^\mu(\phi(t+s)).$$

This means that if we act with left-translation by an element of the one-parameter subgroup, the vector field X^μ is carried onto itself. To extend X^μ to the entire group, we require that this property holds for all left-translations. That is,

$$L_{g*}X(h) = X(gh).$$

Such a vector field is called a *left-invariant* vector field. We have seen that any one-parameter subgroup defines a left-invariant vector field, and if we have a left-invariant vector field then we can solve the differential equation for a one-parameter subgroup (with the initial condition $\phi(0) = e$). Thus, there is a one-to-one correspondence between one-parameter subgroups and left-invariant vector fields.

This correspondence is made explicit through the exponential map. First, note that a left-invariant vector field is completely determined by a vector $X(e)$, since left-invariance requires $X(g) = L_{g*}X(e)$ for all g. We therefore have a map from the vectors at e, which are said to form the *tangent space* T_eG, to left invariant vector fields, and then a map from these vector fields to one-parameter subgroups. We define the exponential map $\exp : T_eG \to G$ by $\exp(v) = \phi_v(1)$, where ϕ_v

is the one-parameter subgroup generated by the left-invariant vector field which takes the value v at e. This has a property we might expect from the exponential: since

$$\left.\frac{d\phi_v(at)}{dt}\right|_{t=0} = a\left.\frac{d\phi_v(t)}{dt}\right|_{t=0} = av,$$

we have $\exp(av) = \phi_{av}(1) = \phi_v(a)$.

Example 2.6. Consider the one-parameter subgroup of $SO(3)$ described above,

$$\phi(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Find the vector $v \in T_eSO(3)$ which generates it, and show that $\phi(\theta) = \exp(\theta v)$, where exp is treated as the usual matrix exponential. For matrix groups, it is always the case that the exp map is nothing more than the matrix exponential.

Solution: To find the vector v, we simply substitute $\phi(\theta)$ into the differential equation connecting one-parameter subgroups and vector fields. We find

$$v = X(e) = \left.\frac{d\phi(\theta)}{d\theta}\right|_{\theta=0} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

To find the exponential of this matrix, we use the series expansion

$$\exp(\theta v) = I + \theta v + \frac{\theta^2}{2!}v^2 + \dots.$$

Since

$$v^2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

we can construct series for each nonzero component:

$$\exp(\theta v)_{11} = \exp(\theta v)_{22} = 1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \ldots = \cos\theta,$$
$$\exp(\theta v)_{21} = -\exp(\theta v)_{12} = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \ldots = \sin\theta.$$

We thus find the expected result,

$$\exp(\theta v) = \phi(\theta).$$

For $SO(3)$, it is clear that the exponential map is surjective. Every element of $SO(3)$ is a rotation by some angle about some axis, and we can define a one-parameter subgroup of rotations about any axis. It is tempting to conclude that the exponential map is always surjective, but this is not

necessarily the case. It is important to be aware of this caveat, because it is the reason that Lie groups are not completely characterized by the vector space T_eG. Nonetheless, the study of this vector space is very useful, and will lead us to the concept of a Lie algebra.

We first introduce the Lie derivative of tensor fields. The Lie derivative is essentially a directional derivative on a manifold; it tells us how a tensor changes if we move in the direction of a particular flow, defined by a vector field. The Lie derivative of the tensor field T along the vector field X is denoted $\mathcal{L}_X T$. We already have the tools to define it. Recall that a vector field X creates a flow $\phi_X(t)$, and that the pushforward map ϕ_{X*} moves tensors along that flow. In order to compare a tensor at p with a tensor at $p + X\epsilon$, we should use the reverse flow, to bring the tensor at $p + X\epsilon$ back to p. We thus define the Lie derivative as

$$\mathcal{L}_X T = \frac{d}{dt}\left(\phi_X(-t)T\right)\Big|_{t=0}.$$

If we take the Lie derivative of a vector field Y along another vector field X, we obtain a third vector field. The result is known as the *Lie bracket* of X and Y, and is denoted by $[X, Y] \equiv \mathcal{L}_X Y$. We can use the coordinate form of the pushforward to find the components of the Lie bracket. By definition,

$$[X, Y] = \frac{d}{dt}\left(\phi_X(-t)Y\right)\Big|_{t=0},$$

so

$$\begin{aligned}[X, Y]^i &= \frac{d}{dt}\left(Y^j(p + tX)\frac{\partial \phi^i(-t)}{\partial x^j}\right)\Big|_{t=0} \\ &= X^j \partial_j Y^i - Y^j \partial_j X^i.\end{aligned}$$

Note that we have used the relation $X^i = \frac{\partial \phi^i(t)}{\partial t}\Big|_{t=0}$.

The Lie bracket has three basic properties which are important. Two are obvious from its coordinate form: antisymmetry, meaning $[X, Y] = -[Y, X]$, and linearity, meaning $[aX_1 + bX_2, Y] = a[X_1, Y] + b[X_2, Y]$. The other is not obvious, but straightforwardly verifiable. It is known as the Jacobi identity:

$$[[X, Y], Z] + [[Z, X], Y] + [[Y, Z], X] = 0.$$

For a matrix group, the Lie bracket is simply the commutator of matrices, $[X, Y] = XY - YX$.

The Lie bracket defines, in essence, a product of two vectors. This gives the set of all vector fields on a manifold the structure of an algebra (roughly, a vector space with a rule for multiplying vectors). This is interesting, but not so much for our purposes. What we will find useful is the fact that left-invariant vector fields are closed under the Lie bracket, so that they form an algebra as well. This holds simply because $L_{g*}[X, Y] = [L_{g*}X, L_{g*}Y] = [X, Y]$. The set of left-invariant vector fields, with the product given by the Lie bracket, is the *Lie algebra* associated to a Lie group. It is conventionally written with lowercase gothic letters, such as $\mathfrak{g}$ for G.

Since a left-invariant vector field is determined by a single vector in T_eG, we can understand all the elements of the Lie algebra by looking at a basis $\{X_i\}$ of T_eG. The elements of this basis are called *generators* of the Lie group. There are as many generators as the dimension of the manifold

of G. The algebra is determined by the Lie brackets $[X^i, X^j]$. These brackets will be vector fields with values at e, which can be written in terms of the generators, so we have

$$[X_i, X_j] = c_{ij}{}^k X_k.$$

The numbers $c_{ij}{}^k$ are called the *structure constants* of the algebra.

Example 2.7. For the algebra $\mathfrak{so}(3)$ of the group $SO(3)$, the fields corresponding to rotations about the three axes form a basis for the three-dimensional group manifold. Find the structure constants of $\mathfrak{so}(3)$.

Solution: We have already found that the tangent vector associated with rotations about the z axis is

$$X_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Similarly, we find

$$X_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad X_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

The Lie brackets of these matrices are their commutators. For example,

$$[X_1, X_2] = X_1 X_2 - X_2 X_1 = X_3.$$

This gives the structure constants $c_{12}{}^1 = c_{12}{}^2 = 0$ and $c_{12}{}^3 = 1$. Likewise, $[X_2, X_3] = X_1$ and $[X_3, X_1] = X_2$. The structure constants are in fact equal to the Levi-Civita symbol, $c_{ij}{}^k = \epsilon_{ij}{}^k$.

The previous example shows that the generators of $SO(3)$ also span the set of antisymmetric 3×3 matrices, so $\mathfrak{so}(3)$ is simply the set of these matrices. This is true more generally; $\mathfrak{so}(n)$ is the algebra of antisymmetric $n \times n$ matrices. To prove this, we note that an element $g \in SO(n)$ can be written as $g = \exp(X)$, where $x \in \mathfrak{so}(n)$. But $g \in SO(n)$ means $gg^\top = I$, so $\exp(X)\exp(X^\top) = I$. Expanding this in powers of X, we have

$$\exp(X)\exp(X^\top) = (1 + X + \ldots)(1 + X^\top + \ldots) = 1 + (X + X^\top) + \ldots = 1.$$

In order for this to be true term-by-term, we must first have $X = -X^\top$, which means X is antisymmetric.

Example 2.8. Show that $SU(2)$, the group of special unitary matrices in $GL(2, \mathbb{C})$, has the same Lie algebra as $SO(3)$.

Solution: We first need to determine a set of generators of $SU(2)$. If $g \in SU(2)$ the $gg^\dagger = 1$, so if $g = \exp(X)$ then $1 + (X + X^\dagger) = 1$, and thus $X = -X^\dagger$. This means that X is anti-Hermitian. Additionally, $\det g = 1$, which means $\operatorname{tr} X = 0$ (through the identity $\det\exp(X) = \exp(\operatorname{tr} X)$). A 2×2 traceless anti-Hermitian matrix has the form

$$X = \begin{pmatrix} ai & b + ci \\ -b + ci & -ai \end{pmatrix},$$

so the generators are

$$X_1 = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \qquad X_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad X_3 = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

Computing commutators, we find

$$[X_1, X_2] = 2X_3, \qquad [X_2, X_3] = 2X_1, \qquad [X_3, X_1] = 2X_2.$$

Therefore, using $Y_i = \frac{1}{2}X_i$ as the generators, we find the exact same structure constants as in $\mathfrak{so}(3)$, which shows that $\mathfrak{so}(3) \simeq \mathfrak{su}(2)$.

3 Physical Observables as Operators

After perusing Sections 1 and 2, a similarity should become apparent. The Lie bracket, which defines a Lie algebra, satisfies three essential conditions, which we review here:

- Antisymmetry: $[X, Y] = -[Y, X]$
- Linearity: $[aX_1 + bX_2, Y] = a[X_1, Y] + b[X_2, Y]$
- Jacobi identity: $[[X, Y], Z] + [[Z, X], Y] + [[Y, Z], X] = 0$

The Poisson bracket in classical mechanics clearly satisfies the first two of these conditions. The Jacobi identity is thornier, but the Poisson bracket does in fact satisfy it as well. To show this, we compute

$$\begin{aligned}
((X, Y), Z) &= \left(\sum_{i=1}^{n} \frac{\partial X}{\partial x^i}\frac{\partial Y}{\partial p_i} - \frac{\partial X}{\partial p^i}\frac{\partial Y}{\partial x_i}, Z \right) \\
&= \sum_{j=1}^{n} \left[\frac{\partial}{\partial x^j} \left(\sum_{i=1}^{n} \frac{\partial X}{\partial x^i}\frac{\partial Y}{\partial p_i} - \frac{\partial X}{\partial p^i}\frac{\partial Y}{\partial x_i} \right) \frac{\partial Z}{\partial p_j} - \frac{\partial}{\partial p^j} \left(\sum_{i=1}^{n} \frac{\partial X}{\partial x^i}\frac{\partial Y}{\partial p_i} - \frac{\partial X}{\partial p^i}\frac{\partial Y}{\partial x_i} \right) \frac{\partial Z}{\partial x_j} \right] \\
&= \sum_{i,j=1}^{n} \left(\frac{\partial^2 X}{\partial x^i \partial x^j}\frac{\partial Y}{\partial p_i}\frac{\partial Z}{\partial p_j} + \frac{\partial X}{\partial x^i}\frac{\partial^2 Y}{\partial p_i \partial x^j}\frac{\partial Z}{\partial p_j} + \frac{\partial^2 X}{\partial p^i \partial p^j}\frac{\partial Y}{\partial x_i}\frac{\partial Z}{\partial x_j} + \frac{\partial X}{\partial p^i}\frac{\partial^2 Y}{\partial x_i \partial p^j}\frac{\partial Z}{\partial x_j} \right. \\
&\qquad \left. - \frac{\partial^2 X}{\partial p^i \partial x^j}\frac{\partial Y}{\partial x_i}\frac{\partial Z}{\partial p_j} - \frac{\partial X}{\partial p^i}\frac{\partial^2 Y}{\partial x_i \partial x^j}\frac{\partial Z}{\partial p_j} - \frac{\partial^2 X}{\partial x^i \partial p^j}\frac{\partial Y}{\partial p_i}\frac{\partial Z}{\partial x_j} - \frac{\partial X}{\partial x^i}\frac{\partial^2 Y}{\partial p_i \partial p^j}\frac{\partial Z}{\partial x_j} \right)
\end{aligned}$$

By associating similar terms of opposite sign, it is fairly easy to see that by adding all cyclic permutations, the result vanishes.

This indicates that it is perhaps worthwhile to view the Poisson bracket structure in classical mechanics as a Lie algebra. This idea has a natural interpretation in terms of Noether's theorem. We constructed conserved quantities from continuous symmetries of the action, and we showed that these quantities generate their respective symmetries through the Poisson bracket. The continuous

symmetries comprise a Lie group, and the generators of the associated Lie algebra can be taken to be the conserved quantities associated with these symmetries.

In Examples 2.7 and 2.8, we explicitly determined the generators of two Lie algebras (which turned out to be isomorphic) as matrices. This was natural, since we were constructing a Lie algebra given a Lie group, and the Lie groups were both given as subgroups of matrix groups ($SO(3) \subset GL(3,\mathbb{R})$ and $SU(2) \subset GL(2,\mathbb{C})$). However, even when matrices for the generators of the algebra are not so readily available, we can hope to find matrices satisfying the commutation relations of the algebra. That is, given the structure constants ${c_{ij}}^k$, we can hope to find matrices $\{A_i\}$ such that

$$[A_i, A_j] = {c_{ij}}^k A_k.$$

This is called a representation of a Lie algebra. It is analogous to a representation of a group: we are mapping an algebraic structure to matrices, such that the matrices embody the algebraic structure.

We will seek a representation of the Lie algebra defined by the Poisson bracket. This will be given by a mapping from physical quantities to linear operators, such that the commutators of the linear operators agree with the Poisson brackets of their respective physical quantities.

Before we proceed, we should take stock of what we are doing. The simple answer is building quantum mechanics, but pretend we don't know this. By following our noses, we have realized that the Poisson bracket satisfies the properties of a Lie bracket, meaning that there is effectively a Lie algebra for classical mechanics, corresponding to the symmetries of classical mechanics. Since Lie algebras have representations, we can determine such a representation for the Lie algebra in classical mechanics. In this representation, each physical quantity will have an associated operator. Linear operators include constant multiples of the identity, which are the analogue of numbers, but they are must richer. Thus, by finding a representation of the Lie algebra given by the Poisson bracket, we will enrich the mathematical structure of classical mechanics while preserving its symmetry.

3.1 Canonical Commutation Relations

For the sake of simplicity and explicitness, we will work in one spatial dimension. We saw in Section 1 that in some sense the most important Poisson bracket is $(x,p) = 1$. However, this also presents a significant challenge for forming a representation. When the trace is defined, the trace of a commutator always vanishes, since

$$\operatorname{tr}(AB) = \sum_{i=1}^{n} (AB)_{ii} = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{ij} B_{ji} \right) = \sum_{j=1}^{n} \left(\sum_{i=1}^{n} B_{ji} A_{ij} \right) = \operatorname{tr}(BA).$$

However, in order to form a representation, we need operators $\hat{x}$ and $\hat{p}$ such that $[\hat{x}, \hat{p}] = \hat{1}$. Since $\operatorname{tr} \hat{1} = n$, this appears to be impossible.

Impossibility results are only as strong as their assumptions, and in this case the assumption was that the trace is defined. The trace is not necessarily defined for linear operators on spaces of infinite dimensions, since the trace involves an infinite sum which may fail to converge. Thus, we have shown that the representation we seek must be infinite dimensional.

Infinite dimensional vector spaces are in many ways like their finite dimensional counterparts. Linear operators act on vectors, have eigenvalues and eigenvectors, and so on. The only difference is that this abstract machinery is being used for vectors which cannot be written as finite lists of numbers. In an infinite dimensional vector space, the vectors have either a countably infinite number of degrees of freedom (such as a sequence of complex numbers), or an uncountable number of degrees of freedom (such as a function $f : \mathbb{R} \to \mathbb{C}$).

We will work primarily with the latter case, function spaces. The inner product on a function space is defined analogously to the inner product in the finite-dimensional case: it is the sum of products of components of the vectors. A "component" of a function is its value at a point, so the inner product is

$$\langle f, g \rangle = \int f(x)\overline{g(x)}\, dx.$$

The adjoint of an operator is defined in terms of the inner product. If $A : V \to V$ is a linear operator on the vector space V, then the adjoint $A^\dagger$ is the operator such that

$$\langle Af, g \rangle = \langle f, A^\dagger g \rangle$$

for all $f, g \in V$. For finite dimensional Euclidean inner product spaces, the adjoint of an operator is given by taking the conjugate transpose of its matrix. In infinite dimensions, the adjoint can be more difficult to construct, as shown in the following example.

Example 3.1. Determine the adjoint of the operator $\frac{d}{dx}$ on the space $C_0^1(\mathbb{R})$ (that is, continuously differentiable functions on $\mathbb{R}$ which go to 0 at infinity).

Solution: Note that after integrating by parts, we have

$$\int_{-\infty}^{\infty} \frac{df}{dx} g\, dx = [fg]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f\, \frac{dg}{dx}\, dx.$$

Since the functions f and g vanish at infinity, the boundary term goes to zero, and so we have

$$\left\langle \frac{df}{dx}, g \right\rangle = \left\langle f, -\frac{dg}{dx} \right\rangle.$$

This establishes that the adjoint of $\frac{d}{dx}$ is $-\frac{d}{dx}$.

We would like to have operators on a function space whose commutator is a constant, to embody the relation $(x, p) = 1$. We will assume both operators are diagonalizable (we will see later that all physical observables map to diagonalizable operators); thus, we are free to make one of the operators diagonal by an appropriate choice of basis. We will choose $\hat{x}$ to be diagonal, meaning that the natural basis of the function space is also an eigenbasis for $\hat{x}$. However, it is not immediately clear what the natural basis is.

The natural basis for a finite-dimensional space is the set of vectors of the form $\langle 0, \ldots, 0, 1, 0, \ldots, 0 \rangle$, that is, vectors with only one nonzero component. Thus, the natural basis for a function space

ought to consist of functions which are only nonzero at one value of x. However, this alone is not quite right. A function such as

$$f(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{otherwise} \end{cases}$$

has norm

$$\|f\|^2 = \langle f, f \rangle = \int |f(x)|^2 \, dx = 0.$$

In fact, function spaces are almost always defined such that $f(x)$ is indistinguishable from zero itself. For an orthonormal basis, we need a function with norm 1. Clearly we cannot obtain this from scaling f. Instead, we define a function $\delta(x)$ such that $\delta(x \neq 0) = 0$ and $\delta(0)$ is infinite, in such a way that

$$\int_{-\infty}^{\infty} \delta(x) \, dx = 1.$$

The set $\{\delta(x - x_0) \mid x_0 \in \mathbb{R}\}$ is appropriate as a basis for the function space, since taking inner products with δ functions extracts components of vectors (i.e., values of functions):

$$\langle f(x), \delta(x - x_0) \rangle = \int f(x)\delta(x - x_0) \, dx = f(x_0).$$

Mathematical aside: The δ function is not a function. It is a *distribution*, meaning it is defined in terms of its action on a smooth test function under an integral. In fact, the relation

$$\int f(x)\delta(x - x_0) \, dx = f(x_0)$$

is a definition of the δ distribution.

A notion of a derivative, called a weak derivative, can be defined on the space of distributions. The weak derivative $\mu'(x)$ of a distribution $\mu(x)$ is the distribution such that, for any smooth test function f,

$$\int \mu'(x) f(x) \, dx = -\int \mu(x) f'(x) \, dx.$$

Note that, if $\mu(x)$ were a differentiable function, this definition would be nothing more than integration by parts. A distribution which formally satisfies a differential equation in terms of weak derivatives is said to be a weak solution to the equation. This notion is important in the theory of partial differential equations.

The Fourier transform of the δ-function is

$$\int_{-\infty}^{\infty} \delta(x - x_0) e^{-ikx} \, dx = e^{-ikx_0}.$$

Taking the inverse Fourier transform gives a useful integral representation of the δ-function:

$$\delta(x - x_0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x - x_0)} \, dk.$$

We will define the action of $\hat{x}$ on $\delta(x - x_0)$ to be

$$\hat{x}\delta(x - x_0) = x_0\delta(x - x_0).$$

By defining the action on all the basis vectors, we have in fact defined the operator $\hat{x}$. To compute $\hat{x}f(x)$, we simply expand f into basis vectors:

$$\hat{x}f(x) = \hat{x}\int \delta(x-y)f(y)\,dy = \int (\hat{x}\delta(x-y))f(y)\,dy = \int y\delta(x-y)f(y)\,dy = xf(x).$$

This reasonable result helps to justify our assumption for the action on the basis vectors.

We now need to determine the action of the operator $\hat{p}$, such that we obtain $[\hat{x},\hat{p}] = 1$. We will appeal here to classical theory. Recall that the Poisson bracket of an arbitrary quantity with the momentum gives the spatial derivative of that quantity:

$$(A,p) = \frac{\partial A}{\partial x}.$$

After converting the quantities to operators and the Poisson bracket to a commutator, this reads

$$[\hat{A},\hat{p}] = \hat{A}\hat{p} - \hat{p}\hat{A} = \frac{\partial A}{\partial x}.$$

This is a differential equation, and we can integrate it. The result, formally, is

$$\hat{A}(x) = e^{-\hat{p}x}\hat{A}(0)e^{\hat{p}x}.$$

We could also write the left hand side as a Taylor expansion around $x = 0$. Since operators act on vectors, the change from $\hat{A}(0)$ to $\hat{A}(x)$ includes both the change in the operator itself and the change in the vector which it acts on. To first order on both sides, we have

$$\hat{A}(0) + x\frac{\partial \hat{A}}{\partial x} - x\hat{A}\frac{\partial}{\partial x} + \mathcal{O}(x^2) = \hat{A}(0) - x\hat{p}\hat{A} + x\hat{A}\hat{p} + \mathcal{O}(x^2),$$

where the minus sign on the left comes from the need to translate vectors by $-x$ back to the origin. Clearly, in order to satisfy this equation, we must have $\hat{p} = -\frac{d}{dx}$. Indeed,

$$\left[x, -\frac{d}{dx}\right] f = \left(-x\frac{d}{dx} + \frac{d}{dx}x\right) f = -x\frac{df}{dx} + x\frac{df}{dx} + f = f,$$

so $[\hat{x},\hat{p}] = 1$.

We have shown that the algebra can be represented on an infinite dimensional space, which is a relief after our initial failure with finite dimensional spaces. However, $[\hat{x},\hat{p}] = 1$ is not quite the algebra we should be seeking to satisfy. There are two concerns, one apparent and one subtle. The apparent concern is that the units do not work out; a commutator has the dimensions of the product of its arguments, so we should have dimensions of $x \cdot p$ (that is, the dimensions of action) on the right hand side. We will insert an arbitrary constant with these dimensions, and strongly foreshadow by labeling this constant $\hbar$. This modifies our result to $\hat{p} = -\hbar\frac{d}{dx}$.

The subtle concern is that, as it stands, $\hat{x}$ and $\hat{p}$ have different properties when taking the adjoint. The operator $\hat{x}$ is its own adjoint; indeed,

$$\langle \hat{x}f, g\rangle = \langle xf, g\rangle = \langle f, xg\rangle = \langle f, \hat{x}g\rangle.$$

We call operators which are their own adjoints *Hermitian* (or, more simply, self-adjoint). However, $\hat{p}$ does not enjoy the same property. In Example 3.1, we showed that the adjoint of $\frac{d}{dx}$ is $-\frac{d}{dx}$, so as it stands, $\hat{p}^\dagger = -\hat{p}$. We say that $\frac{d}{dx}$ is anti-Hermitian.

This is problematic because, continuing with our interpretation of this procedure as generalizing numbers to operators, Hermitian operators are the analogue of real numbers while anti-Hermitian operators are the analogue of pure imaginary numbers. To see this, consider an eigenvalue λ of an (anti-)Hermitian operator A. We then have $A\boldsymbol{v} = \lambda\boldsymbol{v}$ for some vector $\boldsymbol{v}$, and so it follows that

$$\boldsymbol{v}^\top A\boldsymbol{v} = \lambda\boldsymbol{v}^\top\boldsymbol{v}.$$

Note that on each side of this equation we have a number, not a vector or an operator. Taking the adjoint, and using $A^\dagger = \pm A$ (where the signs correspond to Hermitian or anti-Hermitian), we have

$$\pm\boldsymbol{v}^\top A\boldsymbol{v} = \lambda^*\boldsymbol{v}^\top\boldsymbol{v}.$$

If we take the + sign, so that A is Hermitian, we have $\lambda^* = \lambda$ and so eigenvalues are real. If we take the - sign, so that A is anti-Hermitian, then $\lambda^* = -\lambda$ and so eigenvalues are pure imaginary.

It would be more sensible for $\hat{x}$ and $\hat{p}$ to both be Hermitian, so that they are both the operator equivalents of real numbers. However, this is not possible if we demand the commutation relation $[\hat{x}, \hat{p}] = \hbar$. The commutator of two Hermitian operators $\hat{A}$ and $\hat{B}$ is necessarily anti-Hermitian, since

$$[\hat{A}, \hat{B}]^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} = -[\hat{A}, \hat{B}].$$

Thus, if $\hat{x}$ and $\hat{p}$ are both Hermitian, their commutator should be imaginary rather than real. This gives the final necessary modification to the commutation relations: we replace $\hbar$ with $i\hbar$. This changes the representation of p to $\hat{p} = -i\hbar\frac{d}{dx}$, which is Hermitian. The final result is called the *canonical commutation relation*:

$$\boxed{[\hat{x}, \hat{p}] = i\hbar}.$$

Note that x and p need not refer to Cartesian position and momentum; they can be generalized coordinates in Hamiltonian mechanics. Any canonically conjugate variables will have corresponding operators which obey the canonical commutation relation. In general, the rule for forming a commutation relation from a Poisson bracket is

$$[\hat{A}, \hat{B}] = i\hbar(A, B).$$

Example 3.2. Define the angular momentum operators by $\hat{L}_i = \epsilon_{ijk}\hat{x}_j\hat{p}_k$. Verify the rule above by showing explicitly that these obey the algebra $[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k$.

Solution: Substituting the given definition, we have

$$[\hat{L}_i, \hat{L}_j] = \epsilon_{iab}\epsilon_{jcd}[\hat{x}_a\hat{p}_b, \hat{x}_c\hat{p}_d].$$

In multiple dimensions, the commutation relations for $\hat{x}_i$ and $\hat{p}_i$ are $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$. Thus,

$$\begin{aligned}
[\hat{x}_a\hat{p}_b, \hat{x}_c\hat{p}_d] &= \hat{x}_a\hat{p}_b\hat{x}_c\hat{p}_d - \hat{x}_c\hat{p}_d\hat{x}_a\hat{p}_b \\
&= \hat{x}_a(\hat{x}_c\hat{p}_b - i\hbar\delta_{bc})\hat{p}_d - \hat{x}_c(\hat{x}_a\hat{p}_d - i\hbar\delta_{ad})\hat{p}_b \\
&= i\hbar(\delta_{ad}\hat{x}_c\hat{p}_b - \delta_{bc}\hat{x}_a\hat{p}_d).
\end{aligned}$$

Substituting into the expression above, we find

$$[\hat{L}_i, \hat{L}_j] = i\hbar(\epsilon_{abi}\epsilon_{ajc}\hat{x}_c\hat{p}_b - \epsilon_{bia}\epsilon bdj\hat{x}_a\hat{p}_d),$$

where we have used the cyclic rotation identity $\epsilon_{ijk} = \epsilon_{kij} = \epsilon_{jki}$. We will also need the identity

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}.$$

Using this, we have

$$\begin{aligned}[\hat{L}_i, \hat{L}_j] &= i\hbar(\hat{x}_i\hat{p}_j - \hat{x}_b\hat{p}_b - \epsilon_{bia}\epsilon bdj\hat{x}_j\hat{p}_i + \hat{x}_a\hat{p}_a) \\ &= i\hbar(\hat{x}_i\hat{p}_j - \hat{x}_j\hat{p}_i) \\ &= i\hbar\epsilon_{ijk}\hat{L}_k.\end{aligned}$$

The last equality is not immediately obvious, but you can verify it for yourself.

3.2 Dirac Notation

For the remainder of these notes, we will shift to a notation for linear algebra which was championed by Dirac, called either Dirac notation or bra-ket notation. This notation has many advantages over the usual notation for linear algebra. The most significant advantage is also the simplest: in Dirac notation, the distinction between scalars, vectors, and operators becomes visually clear. This symbolic distinction allows for the use of the same label to denote a scalar and a vector if they are related, which is very useful for associating eigenvectors with their eigenvalues. These material advantages aside, Dirac notation is also ubiquitous in discussions of quantum mechanics, so there is no avoiding it.

Let the vector space of interest be H. We call it H because in quantum mechanics we work specifically with *Hilbert spaces*. Hilbert spaces are a generalization of inner product spaces which extend to infinite dimensions. In addition to the axioms of an inner product space, Hilbert spaces are required to be *complete*. This means, roughly, that any sequence of vectors which get arbitrarily close to one another converge to some vector. The space $\mathbb{Q}$ of rational numbers is not complete, but the space $\mathbb{R}$ of real numbers is complete.

The dual of any vector space V, denoted V^*, is defined to be the space of linear functionals $\phi : V \to \mathbb{C}$. The term "functional" in this context simply means a function from a space to its underlying field of scalars (and in quantum mechanics, we always use $\mathbb{C}$ as the field of scalars). A simple example of a linear functional on an inner product space is

$$\phi_y(x) = \langle x, y\rangle.$$

The linearity of ϕ_y follows from the linearity of the inner product.

Dirac notation is in some sense based on the Riesz representation theorem. The Riesz theorem states that for a Hilbert space H, H^* is composed entirely of functionals of the form ϕ_y for some y. That is, if $\phi \in H^*$ then $\phi(x) = \langle x, y\rangle$ for some fixed y. This establishes an isomorphism $H \simeq H^*$.

Any element $y \in H$ can be associated with $\phi_y \in H^*$, and any $\phi \in H^*$ can be identified as ϕ_y for some $y \in H$.

Finally, we will show the notation. Vectors in H are denoted $|x\rangle$, and corresponding elements of H^* are denoted $\langle x|$. These symbols are called kets and bras respectively (so that together they form a bra-ket, or bracket). The action of a functional $\langle y|$ on a vector $|x\rangle$ is written simply by concatenating the two symbols, $\langle y|x\rangle$. This is simply an inner product, since

$$\langle y|x\rangle = \phi_y(x) = \langle x, y\rangle.$$

The notation $\langle \cdot, \cdot \rangle$ is never used; the Dirac notation $\langle \cdot | \cdot \rangle$ is favored.

Operators and scalars are written without the bra/ket decorations; operators are sometimes given a hat, like $\hat{A}$, to distinguish them from scalars. We will adopt that convention in these notes, though be aware that it is not universal and sometimes only context distinguishes between operators and scalars.

As we remarked in the beginning of this section, Dirac notation provides a clear visual distinction between different types of objects. For example, consider the following expression, written in both "standard" and Dirac notation:

$$\begin{aligned} \text{“Standard”}: &\quad (\boldsymbol{\alpha}^\top)^*(A + \lambda B)\boldsymbol{\beta}(\boldsymbol{\xi}^\top)^* C\boldsymbol{\zeta}, \\ \text{Dirac}: &\quad \langle \alpha | (\hat{A} + \lambda \hat{B}) | \beta \rangle \langle \xi | \hat{C} | \zeta \rangle . \end{aligned}$$

In the top expression, it is not immediately clear whether this is a vector, an operator or functional ready to act on a vector, or a scalar. However, in Dirac notation, there is a simple way to distinguish these possibilities. In most cases the entire expression can be ignored, save for the symbols on the edges. The rules are as follows, and you should consider the examples carefully to ensure you understand the logic for the classification:

$\lvert \cdots \rvert$: operator, e.g. $\lvert\psi\rangle\langle\psi\rvert$	$\lvert \cdots \rangle$: vector, e.g. $\lvert\psi\rangle$
$\langle \cdots \rvert$: functional, e.g. $\langle\psi\rvert$	$\langle \cdots \rangle$: scalar, e.g. $\langle\phi\vert\psi\rangle$.

With these rules in mind, it becomes clear that the expression above is a scalar. Note that there can be exceptions to these guidelines; for example, $\langle a|b\rangle |c\rangle$ is the product of a scalar inner product with a vector, so it is a vector, even though it is enclosed in $\langle\rangle$. It is helpful to look for scalars $\langle \cdots \rangle$ and extract them before seeing what kind of object remains. With a bit of practice, it will be immediately obvious in all cases what sort of object you are looking at.

The labels for vectors are in principle arbitrary, but there are conventions which are important to be aware of. The most common convention is labeling the eigenvectors of an operator by their eigenvalues. For example, elements of the position basis (which we have previously written using the δ-function) are denoted by $|x\rangle$ in Dirac notation. They are the eigenvectors of the operator $\hat{x}$, and so we have the equation

$$\hat{x}\,|x\rangle = x\,|x\rangle\,.$$

Note that "x" is being used in three different ways in this equation: as an operator $\hat{x}$, as a label for a vector $|x\rangle$, and as a scalar x. Such overloading of symbols is common in quantum mechanics.

We have so far highlighted the similarities between finite- and infinite-dimensional spaces. However, this is one glaring difference. In finite dimensions, we can write down a matrix corresponding to an operator, and thus operators can be reduced to grids of numbers. Although this is rarely the best way to think about an operator even in finite dimensions, it is a reassuring tool to have available. In infinite dimensions, we do not have this fallback; certainly we will not be able to write a matrix, at least in the usual sense, for $\frac{d}{dx}$. Instead, we will review here in detail the construction of a matrix from its operator in finite dimensions, in a way which allows us to generalize naturally to infinite dimensions.

In a finite dimensional vector space, we have a finite basis, which we will write as $\{|a_1\rangle, \ldots, |a_n\rangle\}$. We can always orthogonalize a basis (e.g., by the Gram-Schmidt method), so we will assume $\langle a_i|a_j\rangle = \delta_{ij}$. This is useful, because it allows us to easily find the components of a vector in the basis. If

$$|v\rangle = \sum_{i=1}^{n} \alpha_i |a_i\rangle ,$$

then

$$\langle a_j|v\rangle = \sum_{i=1}^{n} \alpha_i \langle a_j|a_i\rangle = \sum_{i=1}^{n} \alpha_i \delta_{ji} = \alpha_j .$$

Thus, $\alpha_i = \langle \alpha_i|v\rangle$, and so

$$|v\rangle = \sum_{i=1}^{n} (\langle a_i|v\rangle) |a_i\rangle = \sum_{i=1}^{n} |a_i\rangle \langle a_i|v\rangle .$$

If we know the action of an operator A on all the basis elements $|\alpha_i\rangle$, then we know the operator. That is, we can compute $A|v\rangle$ for any $|v\rangle$, by expanding $|v\rangle$ into the basis:

$$A|v\rangle = A\left(\sum_{i=1}^{n} |a_i\rangle \langle a_i|v\rangle\right) = \sum_{i=1}^{n} (A|a_i\rangle) \langle a_i|v\rangle .$$

Thus, an operator A is specified by n vectors $A|a_i\rangle$. Moreover, we have already found that a vector $|v\rangle$ is specified by n components $\langle a_i|v\rangle$. Putting these facts together, it follows that an operator A is fully specified by n^2 components $\langle a_i|A|a_j\rangle$.

These components are the components of the matrix A_{ij} for A. To see this, recall that the jth column of A_{ij} gives the components of A acting on the jth basis vector; but this is nothing other than $\langle a_i|A|a_j\rangle$. We thus have $A_{ij} = \langle a_i|A|a_j\rangle$. The left hand side of this equality is explicitly a finite-dimensional matrix, but the right hand side does not care whether the basis $\{|a_i\rangle\}$ is a finite or an infinite set. We refer to the object $\langle a_i|A|a_j\rangle$ as a matrix element, regardless of the cardinality of the basis. If the basis happens to be continuously infinite, we replace $\sum$ with $\int$, but this is merely a matter of notation.

Note that the expression $\langle a_i|A|a_j\rangle$ is also a recipe for computing the matrix element: act with A on $|a_j\rangle$ and then take the inner product with $|a_i\rangle$. We can verify that this works in finite dimensions by taking a simple example, a 3×3 matrix:

$$A_{12} = \langle a_1|A|a_2\rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = A_{12}.$$

Example 3.3. Consider the operator $\frac{d}{dx}$ on a space of differentiable functions of one variable. We will later make use of the plane-wave basis, which in terms of the position basis is

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad (k \in \mathbb{R}).$$

These are orthonormal[1] which in the infinite-dimensional case means $\langle k|k'\rangle = \delta(k-k')$. Find all the matrix elements of $\frac{d}{dx}$ in the plane-wave basis.

Solution: Our goal is to compute the quantity $\left\langle k' \left| \frac{d}{dx} \right| k \right\rangle$ for all k, k'. We can easily differentiate the function:

$$\frac{d}{dx}\left(\frac{1}{\sqrt{2\pi}} e^{ikx}\right) = \frac{ik}{\sqrt{2\pi}} e^{ikx}.$$

In terms of vectors, this means $\left\langle x \left| \frac{d}{dx} \right| k \right\rangle = ik \langle x|k\rangle$, and since this holds for all x, it must be the case that $\frac{d}{dx}|k\rangle = ik|k\rangle$. We then have

$$\left\langle k' \left| \frac{d}{dx} \right| k \right\rangle = \langle k'|ik|k\rangle = ik\delta(k-k').$$

In undergraduate treatments of finite-dimensional vector spaces, it is typical to work almost exclusively in a basis, so that vectors and linear maps are identified with lists and grids of scalars. In this context, no one would suggest to "perform the computation in a basis"; there is no other option. However, Dirac notation is built for abstract vector spaces; equations are not written with respect to a particular basis. This is by far the preferable way to do linear algebra; if there is no reason to do violence unto symmetry by fixing a basis, then violence ought not to be done.

However, anyone who has performed even modest computations in quantum physics knows that such violence is a necessity. Often we understand an operator by determining its matrix elements in some basis, and then when working with this operator it is preferable to work in that same basis. For example, if we know the matrix elements of an operator $\hat{A}$ in the $|\alpha_i\rangle$ basis, then we can use the relation

$$\hat{A}|v\rangle = \sum_i (\langle \alpha_i|v\rangle)\hat{A}|\alpha_i\rangle = \hat{A}\left(\sum_i |\alpha_i\rangle\langle\alpha_i|\right)|v\rangle.$$

The last form shown is an important way to represent the computation in the $|\alpha_i\rangle$ basis. The basis appears as the insertion of the operator $\sum_i |\alpha_i\rangle\langle\alpha_i|$ in the middle of the expression. In fact, whenever a set $\{|\alpha_i\rangle\}$ forms a complete basis this insertion is legal, because

$$|v\rangle = \sum_i \langle\alpha_i|v\rangle|\alpha_i\rangle = \left(\sum_i |\alpha_i\rangle\langle\alpha_i|\right)|v\rangle.$$

Put another way, the inserted operator is nothing more than the identity:

$$\sum_i |\alpha_i\rangle\langle\alpha_i| = I.$$

[1] Be wary of the normalization convention here. We have defined $\langle x|k\rangle$ such that $\langle k|k'\rangle = \delta(k-k')$. However, many texts drop the $(2\pi)^{-1/2}$ in $\langle x|k\rangle$, and so $\langle k|k'\rangle = 2\pi\delta(k-k')$.

In quantum mechanics, we often refer to the manipulation of inserting such a sum as "inserting a complete set." When you see this maneuver, or perform it yourself, you should think of choosing a basis to work in; this is all it means to insert a complete set.

Example 3.4. Consider the translation operator $\hat{T}(a)$, which shifts elements of the position basis: $\hat{T}(a)\,|x\rangle = |x+a\rangle$. Determine the matrix elements $\langle k'|\hat{T}(a)|k\rangle$.

Solution: We have essentially been given the matrix elements of $\hat{T}(a)$ in the position basis; we only need to take the inner product with another vector $|x'\rangle$. The result is

$$\langle x'|\hat{T}(a)|x\rangle = \langle x'|x+a\rangle = \delta(x'-x-a).$$

We need to find the matrix elements of the same operator in a different basis. Following the above discussion, we will perform the change of basis by inserting a complete set. In this case, since we know the operator in the $|x\rangle$ basis, we use this complete set. We have

$$\begin{aligned}
\langle k'|\hat{T}(a)|k\rangle &= \langle k'|\left(\int dx'\ |x'\rangle\langle x'|\right)\hat{T}(a)\left(\int dx\ |x\rangle\langle x|\right)|k\rangle \\
&= \int dx\,dx'\ \langle k'|x'\rangle\langle x'|\hat{T}(a)|x\rangle\langle x|k\rangle \\
&= \frac{1}{2\pi}\int dx\,dx'\,\delta(x'-x-a)e^{i(kx-k'x')} \\
&= \frac{1}{2\pi}\int dx\,e^{i(kx-k'(x+a))} \\
&= e^{-ika}\delta(k-k').
\end{aligned}$$

The last equality makes use of the integral representation of the δ-function given in the Mathematical Aside starting on p. 33.

3.3 Symmetry Operators

Example 3.4 concerned the translation operator $\hat{T}(a)$, which moves vectors in the position basis to the right by a: $\hat{T}(a)\,|x\rangle = |x+a\rangle$. The result was the matrix element $\langle k'|\hat{T}(a)|k\rangle = e^{-ika}\delta(k-k')$, which means $\hat{T}(a)\,|k\rangle = e^{-ika}\,|k\rangle$. This means that elements of the plane-wave basis are eigenvectors of translation.

This is evident if we think of vectors $|\psi\rangle$ in terms of their wavefunctions $\psi(x) = \langle x|\psi\rangle$. The translation operator has the action

$$\hat{T}(a)\psi(x) = \langle x|\hat{T}(a)|\psi\rangle = \langle x|\hat{T}(a)\left(\int dx'\,|x'\rangle\langle x'|\right)|\psi\rangle = \int dx'\delta(x-x'-a)\psi(x') = \psi(x-a).$$

Therefore, eigenvectors of $\hat{T}(a)$ are wavefunctions for which

$$\psi(x-a) = c\psi(x).$$

If adding a to the argument multiplies the function by some constant, then presumably the function is exponential; this can be proven rigorously if we additionally assume $\psi(x)$ is continuous. The only exponential functions which are well-behaved at infinity are complex exponentials, so we take $\psi_k(x) \propto e^{ikx}$, and then $\hat{T}(a)\psi_k(x) = e^{ik(x-a)} = e^{-ika}\psi_k(x)$.

Since the eigenvectors of $\hat{T}(a)$ are $|k\rangle$, we can write $\hat{T}(a)$ in terms of an operator constructed from the plane-wave basis. Let $\hat{k}$ be such that

$$\hat{k}\,|k\rangle = k\,|k\rangle\,.$$

Since $\hat{T}(a)$ has the same eigenvectors as $\hat{k}$, but eigenvalues e^{-ika} instead of k, we can write

$$\hat{T}(a) = e^{-i\hat{k}a}.$$

Readers of Section 2 should find this deeply reminiscent of the exponential map from a Lie algebra to its corresponding Lie group. The translation operator $\hat{T}(a)$ plays the role of an element of a Lie group; in this case the group is isomorphic to $\mathbb{R}$ under addition. The operator $\hat{k}$ (or more precisely, $-i\hat{k}$) plays the role of the left-invariant vector field that generates a one-parameter subgroup, which in this case is the entire group.

On one hand, this was to be expected. We built this formalism by constructing a representation of the algebra defined by the Poisson bracket. Translational symmetry was the simplest example we considered in Section 1, and we saw how every symmetry of the classical Lagrangian leads to a conserved quantity, which in turn generates the symmetry via the Poisson bracket. Since $\hat{x}$ is the operator corresponding to the classical quantity x, we ought to have a corresponding generator of translational symmetry.

However, one component is completely unexpected: the appearance of the wavenumber operator $\hat{k}$ as the generator of translations. The classical picture suggests that the momentum operator $\hat{p}$ should be the generator. To the uninitiated, these two operators appear to be wildly different actors competing for the same role: one associated with the wavenumber of a plane wave, the other associated with the momentum of a particle.

In fact, these operators are nearly identical. Moreover, we have already shown this. In Section 3.1, we found that $\hat{p}$ is related to the derivative operator by

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

In Example 3.3, we found that $\langle k'|\frac{d}{dx}|k\rangle = ik\delta(k-k')$, which means $\frac{d}{dx}\hat{k} = ik\hat{k}$. Combining this with the definition of $\hat{k}$, we have

$$\hat{k} = -i\frac{d}{dx}.$$

Therefore, $\hat{p} = \hbar\hat{k}$. So, in fact, both wavenumber and momentum can generate translations; we simply need to insert the constant $\hbar$ appropriately:

$$\hat{T}(a) = e^{-i\hat{k}a} = e^{-i\hat{p}a/\hbar}.$$

The relationship $\hat{p} = \hbar\hat{k}$ is our first result which is contrary to classical intuition. It is suggestive of the infamous *wave-particle duality*: on the left we have an operator tailored to point particles moving with some momentum p, and on the right we have an operator constructed from plane waves with wavelength $\lambda = 2\pi/k$. In addition to the link between waves and particles, we have a quantitative relationship, which we can write as

$$\lambda = \frac{2\pi\hbar}{p} = \frac{h}{p},$$

where $h = 2\pi\hbar$. This equation gives the de Broglie wavelength of a particle; it was one of the first theoretical results which indicated wave-particle duality.

At this point we can take a slight detour and determine the value of $\hbar = h/2\pi$. If we apply the de Broglie relation to a photon, which has $E = pc$, we have

$$\lambda = \frac{h}{E/c} \implies E = \frac{hc}{\lambda} = hf,$$

where $f = c/\lambda$ is the frequency. This linear relation between the energy and the frequency of photons can be observed experimentally (for example, by ionizing atoms with photons of different known frequencies and observing the kinetic energy of liberated electrons for different frequencies). The proportionality constant is found to be $h = 6.626 \times 10^{-34}\,\mathrm{J \cdot s}$, so $\hbar = 1.055 \times 10^{-34}\,\mathrm{J \cdot s}$.

The translation operator is a simple example of a general phenomenon. When a conserved quantity generates a classical symmetry via the Poisson bracket, its corresponding operator is an exponential generator of a one-parameter family of symmetry operators. More precisely, its corresponding operator is $i\hbar$ times the exponential generator, owing to the factor of $i\hbar$ in the canonical commutation relations. Of course, we do not know yet what it means for a quantity to be conserved in the quantum setting; we will take up this question in Section 5.3.

Symmetry operators are exponentials of observables, with an added factor of $-i/\hbar$ in the exponential, and observables are Hermitian. Putting these facts together, it follows that symmetry operators are *unitary*. A unitary operator is one for which its adjoint is its inverse. If $\hat{A}$ is Hermitian, then $\hat{U} = e^{i\hat{A}}$ is unitary, since

$$\hat{U}^\dagger = e^{-i\hat{A}} = \hat{U}^{-1}.$$

For example, we know that classically, angular momentum is the generator of rotations. For the sake of simplicity, we will consider only $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. The operator for rotation about the z axis by an angle θ is, according to our recipé,

$$\hat{R}_z(\theta) = e^{-i\hat{L}_z\theta/\hbar}.$$

We should verify that this is in fact a rotation operator[2]. Let us label vectors by cylindrical coordinates $|r, \theta, z\rangle$. Then we ought to have

$$\langle r', \theta', z'|\hat{R}_z(\phi)|r, \theta, z\rangle = \delta(r - r')\delta(z - z')\delta(\theta' - \theta - \phi).$$

[2]In quantum mechanics, angular momentum is not the full story. Particles can also have *spin*, a kind of intrinsic angular momentum, which contributes to total angular momentum. Denoting the spin by $\hat{S}$, the generator of rotations is the total angular momentum $\hat{J} = \hat{L} + \hat{S}$. The discussion given here is for a spin-zero particle, for which $\hat{J} = \hat{L}$. For nonzero spin, the distinction between $\hat{J}$ and $\hat{L}$ becomes important.

In terms of wavefunctions, we should have

$$\hat{R}_z(\phi)\psi(r,\theta,z) = \psi(r,\theta-\phi,z),$$

where the wavefunction in cylindrical coordinates is $\psi(r,\theta,z) = \langle r,\theta,z|\psi\rangle$. One way to show this is to compute $\hat{R}_z(\theta)$ explicitly. Using $\hat{p}_x = -i\hbar\frac{d}{dx}$ and $\hat{p}_y = -i\hbar\frac{d}{dy}$, we have

$$\hat{R}_z(\phi) = \exp\left(-\left(x\frac{d}{dy} - y\frac{d}{dx}\right)\phi\right).$$

A series expansion of this operator quickly becomes unwieldy. Instead, we will look at the small angle approximation

$$\hat{R}_z(\delta\phi) = 1 - \left(x\frac{d}{dy} - y\frac{d}{dx}\right)\delta\phi = 1 - \frac{d}{d\theta}\delta\phi.$$

Acting with this operator on a wavefunction gives

$$\hat{R}_z(\phi)\psi(r,\theta,z) = \psi(r,\theta,z) - \delta\phi\partial_\theta\psi(r,\theta,z) = \psi(r,\theta-\delta\phi,z).$$

This is the correct infinitesimal result, and in fact it implies the finite result, since

$$\hat{R}_z(\phi) = \hat{R}_z(\phi/N)^N = \lim_{N\to\infty}\hat{R}_z(\phi/N)^N = \lim_{N\to\infty}(e^{-i\hat{L}_z\phi/N\hbar})^N = e^{-i\hat{L}_z\phi/\hbar}.$$

Example 3.5. Canonical conjugacy is a two-way relationship. Show explicitly that position is a generator of momentum-translations; that is,

$$\langle p'|e^{i\hat{x}\Delta p/\hbar}|p\rangle = \delta(p'-p-\Delta p).$$

The change in sign in the exponential is because $[\hat{p},\hat{x}] = -i\hbar$. Note that, since $\hat{p} = \hbar\hat{k}$, $\hat{p} = \hat{k}$ where $p = \hbar k$.

Solution: Using the hint about the vectors $|p\rangle$, we have

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi}}e^{ipx/\hbar}.$$

We can use this relation to change the basis of the operator $e^{-i\hat{x}\Delta p/\hbar}$:

$$\begin{aligned}
\langle p'|e^{i\hat{x}\Delta p/\hbar}|p\rangle &= \int dx\,dx'\,\langle p'|x'\rangle\,\langle x'|e^{i\hat{x}\Delta p/\hbar}|x\rangle\,\langle x|p\rangle \\
&= \frac{1}{2\pi}\int dx\,dx'\,\langle x'|e^{ix\Delta p/\hbar}|x\rangle\,e^{i(xp-x'p')/\hbar} \\
&= \frac{1}{2\pi}\int dx\,e^{ix\Delta p/\hbar}e^{ix(p-p')/\hbar} \\
&= \frac{1}{2\pi}\int dx\,e^{ix(p-p'+\Delta p)/\hbar} \\
&= \delta(p'-p-\Delta p).
\end{aligned}$$

4 Constructing a State Space

We have learned a great deal about operators and their relation to classical observables. By forming a representation of the Poisson algebra, the real numbers which can be used to describe a classical system have been mapped to Hermitian operators. The commutation relations of these operators are closely related to the Poisson brackets of the classical quantities.

However, we have had much less to say about the vector space on which these operators are defined. Implementing the canonical commutation relations required infinite dimensions, so we have used function spaces as prototypes. We need two things: a more systematic way of building the vector space given the operators which act upon it, and a physical understanding of what the vectors mean. As the title of this section suggests, the vectors in the space will turn out to correspond to physical states.

4.1 Spectral Theorem

There is a surprisingly easy way to find a basis for a vector space given a Hermitian operator on it. The spectral theorem states that the eigenvectors of a Hermitian operator (or, in fact, any operator which commutes with its adjoint) form an orthogonal basis for the space. The precise statement of the theorem is the following.

Theorem 4.1 (Spectral Theorem)**.** Let A be a compact linear operator on a Hilbert space $\mathcal{H}$. If $AA^\dagger = A^\dagger A$, then the eigenvectors of A span $\mathcal{H}$. If in addition $A = A^\dagger$, then eigenvectors of A with distinct eigenvalues are orthogonal, and all the eigenvalues are real.

There are three statements here. The last is simple to prove; in fact, we already did so in Section 3.1. To briefly recall, we repeat the argument here in Dirac notation. If $|v\rangle$ is an eigenvector of A, then $A|v\rangle = \lambda|v\rangle$, and so $\langle v|A|v\rangle = \lambda\langle v|v\rangle$. Taking the adjoint, we have $\langle v|A|v\rangle = \lambda^*\langle v|v\rangle$, and so it follows that $\lambda = \lambda^*$, that is, λ is real.

We can use a very similar argument to prove the second claim, that eigenvectors of a Hermitian operator with distinct eigenvalues are orthogonal. Let $|v_1\rangle$ and $|v_2\rangle$ be eigenvectors of A with eigenvalues λ_1 and λ_2 respectively. Then $A|v_1\rangle = \lambda_1|v_1\rangle$, and so

$$\langle v_2|A|v_1\rangle = \lambda_1\langle v_2|v_1\rangle .$$

Had we started with $A|v_2\rangle = \lambda_2|v_2\rangle$, we would have obtained the similar relation

$$\langle v_1|A|v_2\rangle = \lambda_2\langle v_1|v_2\rangle .$$

In fact, since A is Hermitian, the left hand sides are conjugates of each other: $(\langle v_2|A|v_1\rangle)^\dagger = \langle v_1|A|v_2\rangle$. Thus,

$$\lambda_1\langle v_1|v_2\rangle = \lambda_2\langle v_1|v_2\rangle .$$

If we now assume that $\lambda_1 \neq \lambda_2$, this implies that $\langle v_1|v_2\rangle = 0$, so the two vectors are orthogonal.

The first statement is the most important for our purposes: it says that the eigenvectors span the space, so we can understand the entire vector space by understanding the eigenvectors of an

operator on it. It is also by far the most difficult to prove. The following mathematical aside briefly develops the theory of generalized eigenvectors and uses them to prove the first clause of the spectral theorem in the finite-dimensional case, where we can ignore the definition of "compact." This material is not necessary for understanding the rest of the notes.

Mathematical aside: Every linear operator on a vector space defines two subspaces: the kernel and the image. The kernel of an operator is the set of vectors which it sends to zero:

$$\ker A = \{|v\rangle \in \mathcal{H} \mid A|v\rangle = |0\rangle\},$$

where $|0\rangle$ is the zero vector. The image is the range of the linear map:

$$\operatorname{im} A = \{A|v\rangle \mid |v\rangle \in \mathcal{H}\}.$$

You should prove to yourself that both of these are in fact subspaces of $\mathcal{H}$ for any linear operator A.

The eigenvectors for a given eigenvalue λ are the elements of $\ker(A - \lambda I)$. Every operator on a finite-dimensional space has at least one eigenvector. To prove this, fix a nonzero vector $|v\rangle$, and construct the set $\{|v\rangle, A|v\rangle, \ldots, A^n|v\rangle\}$, where $n = \dim \mathcal{H}$. If $A^m|v\rangle = |0\rangle$ for some $m \leq n$, then $A(A^{m-1}|v\rangle) = |0\rangle$, so $A^{m-1}|v\rangle$ is an eigenvector with eigenvalue 0 and we are done. Otherwise, they are all nonzero, and since their number exceeds the dimension of the space they must be linearly dependent. Thus, there are coefficients $\{a_0, \ldots, a_n\}$ such that

$$(a_0 + a_1 A + \ldots + a_n A^n)|v\rangle = |0\rangle.$$

Consider the associated polynomial $a_0 + a_1 z + \ldots + a_n z^n$. By the fundamental theorem of algebra, this can be factored over the complex numbers into $a_n(z - r_1)\cdots(z - r_n)$. Substituting A for z, we have

$$|0\rangle = a_n(A - r_1 I)\cdots(A - r_n I)|v\rangle.$$

This means that either $a_n = 0$, in which case the smaller set $\{|v\rangle, \ldots, A^{n-1}|v\rangle\}$ is linearly dependent on its own and we can use the same argument on it, or one of the operators $(A - r_i I)$ sent a nonzero vector to zero, meaning it has a nontrivial kernel. In the latter case, one of the r_i must be an eigenvalue, and the vector sent to zero is its eigenvector.

Sometimes, however, one eigenvector is the best we can do. Operators can be found which have only a single eigenvalue and only one associated eigenvector (up to scaling). To find more, we look instead for generalized eigenvectors. A generalized eigenvector is an element of $\ker(A - \lambda I)^k$ for some value of k. In fact, we do not need to check all values of k: when $m > n = \dim \mathcal{H}$, $\ker(A - \lambda I)^m = \ker(A - \lambda I)^n$, so all the generalized eigenvectors are contained in $\ker(A - \lambda I)^n$. To prove this, let $|v\rangle$ be a generalized eigenvector of A, and let ℓ be the smallest value for which $(A - \lambda I)^\ell |v\rangle = 0$. Then consider the set $\{|v\rangle, (A - \lambda I)|v\rangle, \ldots, (A - \lambda I)^{\ell-1}|v\rangle\}$. Let

$$a_0|v\rangle + \ldots + a_{\ell-1}(A - \lambda I)^{\ell-1}|v\rangle = 0.$$

Acting on both sides with $(A - \lambda I)^{\ell-1}$ establishes $a_0 = 0$. Then, acting with $(A - \lambda I)^{\ell-2}$ establishes $a_1 = 0$. Going forth in this way, we can show that all the $a_i = 0$, and this means that these ℓ vectors are linearly independent. This implies $\ell \leq n$.

Generalized eigenvectors span the space. We will show this by induction on the dimension of the space. For $\dim \mathcal{H} = 1$, we are done, since we have shown that every linear operator has at least one eigenvector and this suffices to span a one-dimensional space. Now, assume the statement

holds for dimensions up through $n-1$, and consider a Hilbert space with $\dim \mathcal{H} = n$. We have shown that every operator has at least one eigenvalue; for an operator A on $\mathcal{H}$, let λ be one of its eigenvalues. The operator $(A-\lambda I)^n$ defines two subspaces of $\mathcal{H}$, its kernel and its image. These subspaces have a trivial intersection, since if $|v\rangle \in \operatorname{im}(A-\lambda I)^n$ and $|v\rangle \in \ker(A-\lambda I)^n$, then $|v\rangle = (A-\lambda I)^n |w\rangle$ for some $|w\rangle$, and this implies $|0\rangle = (A-\lambda I)^{2n} |w\rangle$. We have already shown that $\ker(A-\lambda I)^{2n} = \ker(A-\lambda I)^n$, so $(A-\lambda I)^n |w\rangle = |0\rangle$, and hence $|v\rangle = 0$. Additionally, by the rank-nullity theorem,

$$\dim \ker(A-\lambda I)^n + \dim \operatorname{im}(A-\lambda I)^n = n.$$

Therefore any vector can be written as a sum of a vector in $\ker(A-\lambda I)^n$ and a vector in $\operatorname{im}(A-\lambda I)^n$. Moreover, λ is an eigenvalue of A, so $\ker(A-\lambda I)^n$ has dimension at least one, meaning $\dim \operatorname{im}(A-\lambda I)^n < n$. We can apply the inductive hypothesis to $\operatorname{im}(A-\lambda I)^n$, showing that it is spanned by generalized eigenvectors of A, and the remainder of the space is $\ker(A-\lambda I)^n$, which is by definition composed of generalized eigenvectors. Thus, $\mathcal{H}$ is spanned by generalized eigenvectors.

Now, to prove the spectral theorem, we show that generalized eigenvectors coincide with regular eigenvectors when A is a normal map. Let A be normal, and let $|v\rangle \in \ker(A-\lambda I)^n$. Then $(A-\lambda I)^n |v\rangle = |0\rangle$. Thus, its norm is zero. We can write this as

$$\langle v|(A^\dagger - \lambda I)^{n-1}(A^\dagger - \lambda I)(A-\lambda I)(A-\lambda I)^{n-1}|v\rangle = 0.$$

Since A is normal, we can commute the two operators in the middle, and obtain

$$\langle v|(A^\dagger - \lambda I)^{n-1}(A-\lambda I)(A^\dagger - \lambda I)(A-\lambda I)^{n-1}|v\rangle = 0.$$

This establishes that $(A^\dagger - \lambda I)(A-\lambda I)^{n-1} |v\rangle = |0\rangle$. Therefore, any inner product with it is zero, such as

$$\langle v|(A^\dagger - \lambda I)^{n-2}(A^\dagger - \lambda I)(A-\lambda I)^{n-1}|v\rangle = 0.$$

But this is simply saying that $(A-\lambda I)^{n-1} |v\rangle = |0\rangle$, and so $|v\rangle \in \ker(A-\lambda I)^{n-1}$. By induction, we have $|v\rangle \in \ker(A-\lambda I)$, so $|v\rangle$ is an eigenvector.

To recap: we have shown that for any operator, its generalized eigenvectors span the space. We then showed that for a normal operator, every generalized eigenvector is a true eigenvector. This implies that the eigenvectors of any normal operator span the space, which is the first clause of the spectral theorem.

The spectral theorem gives rise to a decomposition for operators called the spectral decomposition. Let A be Hermitian, so that its eigenvectors are orthogonal and span the space. Denote these eigenvectors by $|\alpha_i\rangle$ with eigenvalues λ_i. Then, by inserting a complete set to write A in its eigenbasis, we have

$$A|v\rangle = A\left(\sum_i |\alpha_i\rangle\langle\alpha_i|\right)|v\rangle = \left(\sum_i \lambda_i |\alpha_i\rangle\langle\alpha_i|\right)|v\rangle.$$

Thus,

$$A = \sum_i \lambda_i |\alpha_i\rangle\langle\alpha_i|.$$

In infinite dimensions, we have a similar relation, but its exact form is complicated by the fact that the set of eigenvalues of A, also known as the *spectrum* of A, may have both continuous and

discrete parts, so neither a sum nor an integral over eigenvalues is appropriate. Instead, we index the eigenvalues and eigenvectors by a general index set I, and define projection operators by

$$P_\lambda = \sum_{i \in I; \lambda_i \leq \lambda} |\alpha_i\rangle \langle \alpha_i| .$$

The spectral decomposition can then be written as

$$A = \int_{-\infty}^{\infty} \lambda \, dP_\lambda.$$

This is a Riemann-Stieltjes integral; if you are not familiar with this type of integral, disregard this last equation, and instead think heuristically of $A = \sum_i \lambda_i |\alpha_i\rangle \langle \alpha_i|$.

4.2 Complete Sets of Commuting Observables

With the spectral theorem, we can use a Hermitian operator to build a basis for the Hilbert space it acts upon. For example, using the operator $\hat{x}$, we can construct the basis of eigenvectors $\{|x\rangle\}$ for which $\hat{x}|x\rangle = x|x\rangle$.

However, the problem is not this simple. While we do in principle have a set of vectors which span the space, we have said nothing about the uniqueness of these vectors. For a given eigenvalue x, how many vectors satisfy $\hat{x}|x\rangle = x|x\rangle$? There may be a many-dimensional space of such vectors, in which case the mere label $|x\rangle$ is insufficient to pick out a vector.

To alleviate this difficulty, we can apply the spectral theorem to a collection of operators, using simultaneous eigenvectors of all of them as a basis. These eigenvectors can be labeled by the eigenvalues for each operator. The operators each thread through the Hilbert space in some direction, and so together they can delineate the space with a finer resolution, much like a coordinate grid delineates physical space.

Following the analogy of a coordinate system, there ought to be compatibility conditions on the operators we choose. For example, if we tried to use the coordinates (x, y, y^2) for Euclidean 3-space, we would be in a troublesome situation: y and y^2 cannot be specified independently, so points such as $(1, 2, 5)$ would simply not exist. Likewise, imagine attempting to add the momentum operator $\hat{p}$ to $\hat{x}$. Then the basis should consist of vectors $|x, p\rangle$, with $\hat{x}|x, p\rangle = x|x, p\rangle$ and $\hat{p}|x, p\rangle = p|x, p\rangle$. However, such a vector cannot exist. One way to see this is that eigenvectors of $\hat{p}$ are also eigenvectors of $\hat{T}(a) = e^{-i\hat{p}a/\hbar}$, but no eigenvector of position could simultaneously be an eigenvector of translation.

Another way to see this is that, if we had such a vector $|x, p\rangle$, then we would have

$$\hat{x}\hat{p}|x, p\rangle - \hat{p}\hat{x}|x, p\rangle = (xp - px)|x, p\rangle = 0.$$

However, we know that $[\hat{x}, \hat{p}] = i\hbar$, so this cannot be correct. In fact, commutation relations are key to determining if two operators are compatible for describing a state space. Two operators $\hat{A}$ and $\hat{B}$ can be used together to form a basis if and only if they commute. This is formalized in the following theorem.

Theorem 4.2. Let $\hat{A}$ and $\hat{B}$ be diagonalizable operators on the Hilbert space $\mathcal{H}$. Then there exists a basis of $\mathcal{H}$ consisting of simultaneous eigenvectors of $\hat{A}$ and $\hat{B}$ if and only if $[\hat{A}, \hat{B}] = 0$.

One direction of the proof is evident, and follows the reasoning we used with $\hat{x}$ and $\hat{p}$. If there exists a basis consisting of simultaneous eigenvectors $|a, b\rangle$, then for any vector $|v\rangle$,

$$\hat{A}\hat{B}\,|v\rangle = \hat{A}\hat{B}\left(\sum_{a,b} |a,b\rangle\,\langle a,b|\right)|v\rangle = \left(\sum_{a,b} ab\,|a,b\rangle\,\langle a,b|\right)|v\rangle = \hat{B}\hat{A}\left(\sum_{a,b} |a,b\rangle\,\langle a,b|\right)|v\rangle = \hat{B}\hat{A}\,|v\rangle\,.$$

This implies $\hat{A}\hat{B} = \hat{B}\hat{A}$, so $[\hat{A}, \hat{B}] = 0$.

The other direction is somewhat trickier. We are given that $\hat{A}$ and $\hat{B}$ are diagonalizable, so there exist bases $\{|a\rangle\}$ and $\{|b\rangle\}$, satisfying $\hat{A}\,|a\rangle = a\,|a\rangle$ and $\hat{B}\,|b\rangle = b\,|b\rangle$. We will use the commutation of $\hat{A}$ and $\hat{B}$ to establish that these operators respect each other's eigenspaces; that is, $\hat{A}$ sends eigenvectors of $\hat{B}$ to eigenvectors with the same eigenvalue, and vice-versa. This is quite easy to show:

$$\hat{A}(\hat{B}\,|a\rangle) = \hat{B}\hat{A}\,|a\rangle = a(\hat{B}\,|a\rangle),$$

so both $|a\rangle$ and $\hat{B}\,|a\rangle$ are eigenvectors of $\hat{A}$ with eigenvalue a.

Using this fact, we can consider $\hat{B}$ restricted to of the eigenspaces of $\hat{A}$ separately. For each eigenvalue of $\hat{A}$, we have a space of eigenvectors with some dimension, and $\hat{B}$ maps this space into itself by the argument above. Since there is a basis of eigenvectors of $\hat{B}$ for the entire space, we can restrict this basis to the eigenspace of $\hat{A}$, thereby obtaining a set of vectors with a fixed eigenvalue a under $\hat{A}$ and various eigenvalues b under $\hat{B}$. Repeating this process for each eigenspace of $\hat{A}$, we obtain our basis of vectors $|a, b\rangle$.

In order to fully characterize a Hilbert space, we would like to have enough operators in our set that their eigenvalues uniquely select a simultaneous eigenvector. Such a set is called a *complete set of commuting observables*. Given a finite complete set of commuting observables $\{\hat{A}_1, \ldots, \hat{A}_n\}$, we can build a basis of vectors $|a_1, \ldots, a_n\rangle$, where the eigenvalues a_i may have to satisfy compatibility conditions.

Of course, there is a dilemma here: if we do not know the Hilbert space *a priori*, how can we decide whether a set of observables is complete? It turns out that this is a decision we are permitted to make ourselves on physical grounds, and then require the Hilbert space to comply. For example, if we are studying a single particle in one dimension, then classically the particle is characterized by a position and a velocity, or equivalently, a position and a momentum. We might like to include both $\hat{x}$ and $\hat{p}$ in our complete set, but these do not commute, so we must settle for only one of them. In fact, if we choose either operator to be our (singleton) complete set, the Hilbert space is large enough to encode both position and momentum. Explicitly, if we work in the $\hat{x}$ eigenbasis then we have momentum eigenstates

$$|p\rangle = \int dx\ \langle x|p\rangle\,|x\rangle = \frac{1}{\sqrt{2\pi}}\int dx\, e^{ipx/\hbar}\,|x\rangle\,.$$

Likewise, if we work in the $\hat{p}$ eigenbasis then we have position eigenstates

$$|x\rangle = \int dp\ \langle p|x\rangle\,|p\rangle = \frac{1}{\sqrt{2\pi}}\int dp\, e^{-ipx/\hbar}\,|p\rangle\,.$$

We can apply the same principles to more particles and more dimensions. In general, a classical system of N particles in d dimensions is characterized by $2Nd$ variables, which can be taken to be Nd position variables and Nd momentum variables. These come in conjugate pairs, and the corresponding operators do not commute, so we can only take one of each. We are technically free to make independent choices for each pair, but there is usually little good reason to mix position and momentum observables, so more commonly we make a uniform choice. Then we have two potential complete sets of commuting observables:

$$\{\hat{x}_1^1, \ldots, \hat{x}_d^1, \ldots, \hat{x}_1^N, \ldots, \hat{x}_d^N\} \quad \text{and} \quad \{\hat{p}_1^1, \ldots, \hat{p}_d^1, \ldots, \hat{p}_1^N, \ldots, \hat{p}_d^N\}.$$

The bases of simultaneous eigenvectors for these sets are (naturally) called the position basis and momentum basis respectively. They are two different bases for the same Hilbert space. Later on, we will show how to construct a basis that is tailored to a particular physical system. In fact, constructing a basis will constitute a solution of the system.

4.3 Vectors as Physical States

We have constructed operators explicitly out of classical variables, so it is clear that these operators have a connection to physics. However, the underlying Hilbert space came about simply because the operators needed some space to act upon. The physical interpretation of vectors in the Hilbert space is more difficult to see. We will show now that the vectors actually correspond to the physical states of a system. This understanding will allow us to prove the uncertainty principle, which puts a quantitative limit on the precision with which two quantities can be simultaneously realized by a system.

Our first hint that vectors are physical states came in the last section, when we constructed bases out of complete sets of commuting observables. For the sake of being explicit, consider a single particle in three dimensions, for which a complete set of commuting observables is $\{\hat{x}, \hat{y}, \hat{z}\}$. Then the basis consists of vectors $|x, y, z\rangle$, satisfying

$$\hat{x}\,|x, y, z\rangle = x\,|x, y, z\rangle\,, \quad \hat{y}\,|x, y, z\rangle = y\,|x, y, z\rangle\,, \quad \hat{z}\,|x, y, z\rangle = z\,|x, y, z\rangle\,.$$

Each basis vector corresponds to a point in $\mathbb{R}^3$ where the particle could be. Thus, we might posit that each of these basis vectors represents a state in which the system is at the corresponding point. This vague notion raises several questions, which we will treat in increasing order of difficulty.

The first question is normalization. Recall that an eigenvector is really a one-dimensional space; if $|v\rangle$ is an eigenvector of an operator $\hat{A}$, then so is $\alpha\,|v\rangle$ for any $\alpha \in \mathbb{C}$. Given this, how are we to decide which vector proportional to $|x, y, z\rangle$ corresponds to a state with the particle at position (x, y, z)? The answer is simple: we remove the degeneracy by dealing only with vectors of length 1. That is, we require $\langle x, y, z|x, y, z\rangle = 1$.

However, this isn't a complete answer; some degeneracy remains. Let $|\psi\rangle = e^{i\phi}\,|x, y, z\rangle$; then $|\psi\rangle$ has the same eigenvalues for $\hat{x}$, $\hat{y}$, and $\hat{z}$, and moreover $\langle\psi|\psi\rangle = \langle x, y, z|e^{-i\phi}e^{i\phi}|x, y, z\rangle = \langle x, y, z|x, y, z\rangle = 1$. Thus, our normalization condition does not distinguish between vectors which differ by a phase. This is a subtle but deeply important feature of quantum mechanics, which we will deal with more fully in Section 6. For now, it suffices to know that while an overall phase is negligible, the relative phase between vectors is physically important.

The next question is immediate: what about momentum? Classically, a position alone is not a full description of a state; we also need to know the momentum of a particle. However, we have already seen that when a particle is in a position eigenstate, it is not in a momentum eigenstate. If we are to continue to follow our noses at this point, we are forced to break ranks with Newton: our states cannot simultaneously have a definite position and a definite momentum. Indeed, a position eigenstate is a sum over all momentum eigenstates, and vice-versa. This is a first inkling of the uncertainty principle, which we will make more general and more explicit later.

This discussion leads to our final and most difficult question: we can understand the basis vectors in terms of the operators used to construct them, but what about nontrivial linear combinations, or *superpositions*, of these basis vectors? Consider a particle in one dimension, with the basis $\{|x\rangle\}$. An arbitrary vector $|\psi\rangle$ can be written, as we have seen, in terms of a wavefunction:

$$|\psi\rangle = \int dx\ |x\rangle \langle x|\psi\rangle = \int dx\, \psi(x)\, |x\rangle\,.$$

We now have the added condition that physical states correspond to normalized vectors, so

$$\langle\psi|\psi\rangle = \int dx\ \langle\psi|x\rangle \langle x|\psi\rangle = \int dx\, |\psi(x)|^2 = 1.$$

The function $|\psi(x)|^2$ has some interesting properties. We have just seen that it integrates to 1; it is also nonnegative, since it is the square of the magnitude of a complex number. These are the properties that must be satisfied by a probability distribution.

If we take this suggestion seriously, then $|\psi(x)|^2 = |\langle x|\psi\rangle|^2$ is the probability density for finding a particle in the state $|\psi\rangle$ at the position x. Naturally, if $|\psi\rangle = |x_0\rangle$, then $|\psi(x)|^2 = 0$ for any $x \neq x_0$, in line with our interpretation of $|x_0\rangle$ as a definite state of position. However, if $|\psi\rangle$ is not a definite state of position, then the particle has nonzero probabilities of being found at more than one position.

Of course, there is nothing special about position or the position basis. The more general statement we should be making is about the inner product of any two states: $|\langle\phi|\psi\rangle|^2$ is the probability of finding the state $|\psi\rangle$ in the state $|\phi\rangle$. If the states are orthogonal, meaning $\langle\phi|\psi\rangle = 0$, then it is impossible to measure a system in state $|\psi\rangle$ and find that it is in $|\phi\rangle$. However, in any other case, there is a nonzero probability of this happening.

This all alludes to the fact that measurement is necessarily an active process. Even if a particle starts out in a superposition of positions, if we measure its position we will obtain one value. After the measurement, the particle really will be in that position, and only that position; we say the superposition is collapsed by the measurement. More generally, if we measure the value of some observable corresponding to an operator $\hat{A}$, with spectrum $\{\alpha_i\}$, then we will obtain one of the eigenvalues α_i. The probability of obtaining a particular eigenvalue is given by $|\langle\alpha_i|\psi\rangle|^2$, and the normalization of $|\psi\rangle$ ensures that these probabilities sum to 1. After the measurement, the system is no longer in state $|\psi\rangle$, but rather in the state $|\alpha_i\rangle$.

The claims we are making seem preposterous. The interpretation we have given of the state space implies that a particle cannot simultaneously have definite position and momentum; that a particle can be in a probabilistic superposition of different classical states; and that measuring the value of an observable necessarily changes a system into a definite state of that observable. Nonetheless,

the predictions of quantum mechanics have been verified to stunning accuracy whenever they have been put to the test. Preposterous though they may be, these claims are true.

For the sake of some credibility, we will describe one simple example in which the reality of quantum superpositions can be demonstrated. In addition to their frequency (or energy), photons have a degree of freedom called polarization. Classically, the polarization is interpreted as the direction of electric field oscillations in the electromagnetic wave. A polarization filter is a piece of material which only permits light polarized in one direction to pass through. Polarization filters are inexpensive and common; sunglasses are typically polarized to filter out glare reflected from roads.

A polarization filter can be considered a crude apparatus for measuring polarization. It can be represented by an operator with two eigenstates: one which is the polarization direction that the filter accepts, and one which is the orthogonal polarization. For example, if we have a horizontal polarization filter, then it transmits the horizontally polarized state $|\rightarrow\rangle$ and blocks the vertically polarized state $|\uparrow\rangle$. These two states can be taken as a basis for the state space.

Naturally, if we place a vertical filter on top of a horizontal filter, no light passes through both. Formally, this is because any initial polarization state can be expanded as $|\psi\rangle = \alpha\,|\rightarrow\rangle + \beta\,|\uparrow\rangle$. When it reaches the horizontal filter, it has a probability $|\,\langle\rightarrow|\psi\rangle\,|^2 = \alpha^2$ of passing through, and a probability $|\,\langle\uparrow|\psi\rangle\,|^2 = \beta^2$ of being blocked. If it passes through, then it is in state $|\rightarrow\rangle$, and so it will certainly be blocked by the vertical filter. All this makes good classical sense.

Now, consider adding a filter in the middle which transmits light in the state $|\nearrow\rangle = \frac{1}{\sqrt{2}}(|\rightarrow\rangle + |\uparrow\rangle)$. Physically, this filter is just a horizontal filter turned by 45°. Now, after the horizontal filter collapses the initial state into $|\rightarrow\rangle$, it reaches the diagonal filter. The probability of passing through is

$$|\,\langle\nearrow|\rightarrow\rangle\,|^2 = \frac{1}{2}.$$

This half of the horizontally polarized light is then in the state $|\nearrow\rangle$, and impinges on the vertical filter. Again, the probability is

$$|\,\langle\uparrow|\nearrow\rangle\,|^2 = \frac{1}{2}.$$

Thus, a total fraction $\frac{1}{4}\alpha^2$ of the initial light is transmitted. If the initial light is unpolarized then the average value $\langle\alpha^2\rangle = \frac{1}{2}$, so $\frac{1}{8}$ of the intensity passes through all three filters. Adding a filter in the middle of the system allowed light to pass through when none could before; this highlights how measurement changes a state.

Example 4.1. Consider placing $N-1$ filters between the horizontal and vertical filters, which accept light in the states

$$|\theta_k\rangle = \cos\frac{k\pi}{N}\,|\rightarrow\rangle + \sin\frac{k\pi}{N}\,|\uparrow\rangle \qquad (1 \le k \le N-1).$$

Show that in the limit $N \to \infty$, half of the initial intensity is transmitted (meaning that the first filter is the only one which rejects any light).

Solution: We know that half of the initial unpolarized light transmits through the horizontal filter and collapses to the state $|\rightarrow\rangle = |\theta_0\rangle$, so we will start from this point. The probability for

light in the state $|\theta_k\rangle$ to transmit through the next filter is

$$|\langle\theta_{k+1}|\theta_k\rangle|^2 = \left|\cos\frac{k\pi}{N}\cos\frac{(k+1)\pi}{N} + \sin\frac{k\pi}{N}\sin\frac{(k+1)\pi}{N}\right|^2 = \cos^2\frac{\pi}{N},$$

where we have used the cosine difference identity in the last equality. Therefore, the probability for the horizontally polarized light to transmit through all N of the remaining filters is $\cos^{2N}\frac{\pi}{N}$. In the limit $N\to\infty$, this is

$$\begin{aligned}\lim_{N\to\infty}\cos^{2N}\frac{\pi}{N} &= \lim_{N\to\infty}\left(1-\frac{\pi^2}{2N^2}\right)^{2N}\\ &= \lim_{N\to\infty}\left(1-\frac{\pi^2}{N}\right)\\ &= 1,\end{aligned}$$

where we have used the small-angle approximation $\cos\theta\approx 1-\frac{1}{2}\theta^2$ and the binomial approximation $(1+\alpha)^n\approx 1+n\alpha$.

4.4 Uncertainty Principle

We have already seen a very weak form of the uncertainty principle: definite states of position are never definite states of momentum, so it is impossible for a state to have a definite value of position and of momentum simultaneously. We will now explore this idea further, first in the specific case of position and momentum, and then for general observables.

Consider a single particle in one dimension. Its state $|\psi\rangle$ is in general a superposition of many position states, or in an alternative description, a superposition of many momentum states. If the state is a position eigenstate, then it is a superposition of all possible momentum states, and vice-versa. However, superpositions can also be more localized, having their highest amplitude in a small region of position space or momentum space. Even though we cannot exactly localize both position and momentum, we can attempt to find a state which is somewhat localized in both coordinates.

First, we should decide on a way to quantify the uncertainty in a quantity for a given state. Since we have seen that wavefunctions can be squared to give probability distributions, we will use the standard deviation of this distribution. Recall that the standard deviation of a random variable X is

$$\sigma[X] = \sqrt{E[(X-\mu)^2]} = \sqrt{E[X^2]-E[X]^2}.$$

This suggests we should find a way of computing the expected value of a quantity. This is relatively simple. If we have an observable represented by an operator $\hat{A}$, which has spectrum $\{\alpha_i\}$ and corresponding eigenstates $|\alpha_i\rangle$, then any state can be expanded as

$$|\psi\rangle = \sum_i \langle\alpha_i|\psi\rangle\,|\alpha_i\rangle\,.$$

The probability of measuring the value α_i is $|\langle\alpha_i|\psi\rangle|^2$, so the expected value is

$$E[A] = \sum_i \alpha_i |\langle\alpha_i|\psi\rangle|^2 = \langle\psi| \left(\sum_i \alpha_i |\alpha_i\rangle \langle\alpha_i| \right) |\psi\rangle .$$

The sum in the parentheses is the spectral decomposition of $\hat{A}$, so we have $E[A] = \langle\psi|\hat{A}|\psi\rangle$. Thus, the standard deviation is

$$\sigma[A] = \sqrt{\langle\psi|\hat{A}^2|\psi\rangle - (\langle\psi|\hat{A}|\psi\rangle)^2}.$$

We usually denote the standard deviation by ΔA rather than $\sigma[A]$.

Example 4.2. Determine Δx and Δp for the wavefunction

$$\psi(x) = \frac{1}{(2\pi)^{1/4}\sigma^{1/2}} e^{-x^2/4\sigma^2}.$$

Solution: Since we are given the state in the position basis, it is simple to compute Δx. Since $\psi(x) = \psi(-x)$, we have

$$\langle\psi|\hat{x}|\psi\rangle = \int dx\, x|\psi(x)|^2 = 0.$$

The expected value of x^2 is

$$\begin{aligned}
\langle\psi|\hat{x}^2|\psi\rangle &= \int dx\, x^2|\psi(x)|^2 \\
&= \frac{1}{\sqrt{2\pi}\sigma} \int dx\, x^2 e^{-x^2/2\sigma^2} \\
&= \frac{2\sigma^2}{\sqrt{\pi}} \int_0^\infty du\, \sqrt{u} e^{-u} \\
&= \sigma^2.
\end{aligned}$$

Therefore, $\Delta x = \sigma$.

We have already seen that $\hat{p}$ can be represented by $-i\hbar\frac{d}{dx}$ in the position basis, so

$$\begin{aligned}
\langle\psi|\hat{p}|\psi\rangle &= \frac{1}{\sqrt{2\pi}\sigma} \int dx\, e^{-x^2/4\sigma^2} \left(-i\hbar \frac{d}{dx} \right) e^{-x^2/4\sigma^2} \\
&= \frac{i\hbar}{2\sqrt{2\pi}\sigma^3} \int dx\, x e^{-x^2/2\sigma^2} \\
&= 0.
\end{aligned}$$

Following the same procedure for $\hat{p}^2$, we find

$$\begin{aligned}\langle\psi|\hat{p}^2|\psi\rangle &= \frac{1}{\sqrt{2\pi}\sigma}\int dx\, e^{-x^2/4\sigma^2}\left(-i\hbar\frac{d}{dx}\right)^2 e^{-x^2/4\sigma^2} \\ &= \frac{\hbar^2}{2\sqrt{2\pi}\sigma^3}\int dx\,\left(1-\frac{x^2}{2\sigma^2}\right)e^{-x^2/2\sigma^2} \\ &= \frac{\hbar^2}{2\sqrt{2\pi}\sigma^3}\left(\sqrt{2\pi}\sigma-\sqrt{\pi/2}\sigma\right) \\ &= \frac{\hbar^2}{4\sigma^2}.\end{aligned}$$

Therefore, $\Delta p = \frac{\hbar}{2\sigma}$.

The Gaussian wavefunction in Example 4.2 is localized to a region in x-p space with an area of roughly $\Delta x\Delta p = \frac{\hbar}{2}$. It turns out that this is the lowest product achievable; for any wavefunction, $\Delta x\Delta p \geq \frac{\hbar}{2}$.

To prove this, we will start by assuming that $\langle\psi|\hat{x}|\psi\rangle = \langle\psi|\hat{p}|\psi\rangle = 0$. This can always be made the case by acting with the translation operator and the momentum-translation operator defined in Example 3.5. These operators leave the standard deviation invariant; if you wish to be extra careful, you can establish this for yourself.

This assumption simplifies the quantity of interest to

$$\Delta x\Delta p = \sqrt{\langle\psi|\hat{x}^2|\psi\rangle\,\langle\psi|\hat{p}^2|\psi\rangle}.$$

To obtain the desired inequality, we start from the normalization condition and integrate by parts:

$$1 = \int dx\,\psi(x)\psi^*(x) = \int dx\, x(\psi'(x)\psi^*(x)+\psi(x)\psi'^*(x)) = 2\,\mathrm{Re}\left(\int dx\, x\psi'(x)\psi^*(x)\right).$$

The real part of a complex number is less than its magnitude, so

$$1 \leq 4\left|\int dx\, x\psi'(x)\psi^*(x)\right|^2.$$

The integral here can be thought of as the inner product of $\psi'(x)$ and $x\psi(x)$. Using the Cauchy-Schwarz inequality ($|\langle v|w\rangle|^2 \leq \langle v|v\rangle\langle w|w\rangle$), we find

$$1 \leq 4\left(\int dx\,|\psi'(x)|^2\right)\left(\int dx\, x^2|\psi(x)|^2\right).$$

The second factor is $\langle\psi|\hat{x}^2|\psi\rangle$. The first factor can be related to $\langle\psi|\hat{p}^2|\psi\rangle$ with a little manipulation:

$$\langle\psi|\hat{p}^2|\psi\rangle = -\hbar^2\int dx\,\psi^*(x)\psi''(x) = \hbar^2\int dx|\psi'(x)|^2,$$

where in the last equality we integrated by parts. It follows that

$$\frac{\hbar^2}{4} \leq \langle\psi|\hat{p}^2|\psi\rangle\,\langle\psi|\hat{x}^2|\psi\rangle\,,$$

and so $\Delta x \Delta p \geq \frac{\hbar}{2}$.

We can summarize this result in a theorem.

Theorem 4.3 (Uncertainty Principle)**.** For any particle state $|\psi\rangle$, the uncertainties Δx and Δp satisfy

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

This is by far the most well-known uncertainty relation, but it is not the only one. The underlying tension between $\hat{x}$ and $\hat{p}$ was their nonvanishing commutator, which prevents them from sharing any eigenvectors, as we saw in Section 4.2. Other operators which do not commute have similar uncertainty relations.

To show this, we will take two general Hermitian operators $\hat{A}$ and $\hat{B}$, and a general state $|\psi\rangle$. Let

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle \,, \quad \langle \hat{B} \rangle = \langle \psi | \hat{B} | \psi \rangle \,.$$

Then

$$\Delta A = \sqrt{E[(\hat{A} - \langle \hat{A} \rangle)^2]} = \sqrt{\langle \psi | (\hat{A} - \langle \hat{A} \rangle^2 | \psi \rangle},$$

and likewise for ΔB. Defining $|\alpha\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle$ and $|\beta\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle$, we have

$$\Delta A \Delta B = \sqrt{\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle}.$$

The Cauchy-Schwarz inequality then implies that $\Delta A \Delta B \geq |\langle \alpha | \beta \rangle|$. The inner product is

$$\begin{aligned} \langle \alpha | \beta \rangle &= \langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle) | \psi \rangle \\ &= \langle \psi | (\hat{A}\hat{B} - \langle \hat{A} \rangle \hat{B} - \hat{A} \langle \hat{B} \rangle + \langle \hat{A} \rangle \langle \hat{B} \rangle) | \psi \rangle \\ &= \langle \psi | \hat{A}\hat{B} | \psi \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle. \end{aligned}$$

This means $\langle \beta | \alpha \rangle = \langle \psi | \hat{B}\hat{A} | \psi \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$. Now,

$$\Delta A \Delta B \geq |\langle \alpha | \beta \rangle| \geq |\mathrm{Im} \langle \alpha | \beta \rangle| = \left| \frac{\langle \alpha | \beta \rangle - \langle \beta | \alpha \rangle}{2i} \right| = \frac{\left| \langle \psi | [\hat{A}, \hat{B}] \psi \rangle \right|}{2}.$$

This is the general form of the uncertainty relation, called the Robertson uncertainty relation.

Theorem 4.4 (Robertson uncertainty relation)**.** Let $\hat{A}$, $\hat{B}$ be Hermitian operators on a state space $\mathcal{H}$, and let $|\psi\rangle \in \mathcal{H}$. Then the uncertainties ΔA and ΔB satisfy the inequality

$$\Delta A \Delta B \geq \frac{\left| \langle \psi | [\hat{A}, \hat{B}] \psi \rangle \right|}{2}.$$

These results place fundamental limits on the degree to which a state can have well-defined values for two non-commuting observables. This is wholly unlike classical physics, in which a system is assumed to have definite values for all quantities we may be interested in. It is very important to note that nowhere so far in this section have we mentioned a measurement. The uncertainty

principle is often stated as "non-commuting observables cannot be simultaneously measured"; this is true, but it is only a consequence of the actual uncertainty principle, which says that non-commuting observables cannot *be* simultaneously. It is not a question of measuring, but a question of being. The states themselves do not simultaneously have a definite position and a definite momentum, independent of our ability to measure these things.

Example 4.3. You will show in the next section that a particle in a one-dimensional box of length L has a wavefunction

$$\psi_n(x) = \begin{cases} \sqrt{2/L}\sin(\pi n x/L) & \text{if } 0 \le x \le L, \\ 0 & \text{otherwise} \end{cases},$$

where $n = 1, 2, 3, \ldots$. Show that the uncertainty relation is satisfied.

Solution: The average values of position and momentum are

$$\begin{aligned} \langle x \rangle &= \frac{2}{L}\int_0^L dx\, x \sin^2 \frac{\pi n x}{L} = \frac{L}{2}, \\ \langle p \rangle &= \frac{2\pi n}{L^2}\int_0^L dx\, \sin\frac{\pi n x}{L}\cos\frac{\pi n x}{L} = 0. \end{aligned}$$

Therefore,

$$\begin{aligned} (\Delta x)^2 &= \frac{2}{L}\int_0^L dx\,(x - L/2)^2 \sin^2\frac{\pi n x}{L} \\ &= -\frac{L^2}{4} + \frac{2}{L}\int_0^L dx\, x^2 \sin^2\frac{\pi n x}{L} \\ &= -\frac{L^2}{4} + L^2\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right) \\ &= L^2\left(\frac{1}{12} - \frac{1}{2\pi^2 n^2}\right). \end{aligned}$$

Similarly,

$$\begin{aligned} (\Delta p)^2 &= \frac{2\hbar^2\pi^2 n^2}{L^3}\int_0^L dx\, \sin^2\frac{\pi n x}{L} \\ &= \frac{\hbar^2\pi^2 n^2}{L^2}. \end{aligned}$$

Therefore,

$$\Delta x \Delta p = \frac{\hbar}{2}\sqrt{\frac{\pi^2 n^2}{3} - 2}.$$

This quantity is minimized for $n = 1$, when it is $\frac{\hbar}{2}\sqrt{\frac{\pi^2}{3} - 2} > \frac{\hbar}{2}$. Incidentally, since we have already proved the uncertainty relation, this can be taken as a proof that $\pi > 3$.

5 Quantum Dynamics

We have successfully built a mathematical picture in which physical states are vectors and physical quantities are operators on the space of these vectors. We are, at last, at a point where we can stop building the mathematical framework and start to explore the physics.

In our development thus far, we have mostly focused on the representations of position and momentum. These are canonically conjugate, and so momentum is the generator of translations. This idea translated naturally from the classical setting of Poisson brackets to the quantum setting of commutators. We also showed, classically, that the Hamiltonian is the generator of time evolution. We will use this observation to build the Heisenberg picture of quantum dynamics.

The Heisenberg picture makes the relation to classical mechanics very clear, but it is somewhat difficult to compute with. It is more common to solve quantum systems using the Schrödinger picture, which is a different mathematical representation of the same physics. In the Schrödinger picture, it will become clear that solving a quantum system amounts to solving an eigenvalue problem.

5.1 Heisenberg Picture

In Section 1, we showed that

$$\frac{dQ}{dt} = (Q, \mathcal{H}) + \frac{\partial Q}{\partial t},$$

where $\mathcal{H}$ is the Hamiltonian. We constructed quantum operators using the recipe $[\hat{A}, \hat{B}] = i\hbar(A, B)$, so the quantum version of this equation should read

$$\frac{d\hat{Q}}{dt} = -\frac{i}{\hbar}[\hat{Q}, \hat{\mathcal{H}}] + \frac{\partial \hat{Q}}{\partial t},$$

where $\hat{H}$ is the Hamiltonian operator. This is called the Heisenberg equation of motion, and it tells us how every operator associated with a quantum system with given Hamiltonian $\hat{H}$ evolves.

We can actually solve the Heisenberg equation, in a formal sense. By reflecting on the structure of the right hand side, we are led to the solution

$$\hat{Q}(t) = e^{i\hat{\mathcal{H}}t/\hbar}\hat{Q}e^{-i\hat{\mathcal{H}}t/\hbar}.$$

It is simple to verify that this satisfies the equation:

$$\begin{aligned}\frac{d\hat{Q}}{dt} &= \frac{i}{\hbar}\hat{H}\hat{Q}(t) + e^{i\hat{\mathcal{H}}t/\hbar}\frac{\partial \hat{Q}}{\partial t}e^{-i\hat{\mathcal{H}}t/\hbar} - \frac{i}{\hbar}\hat{Q}(t)\hat{H} \\ &= -\frac{i}{\hbar}[\hat{Q}, \hat{H}] + \frac{\partial \hat{Q}}{\partial t}(t).\end{aligned}$$

The Hamiltonian operator can, in many cases, be lifted naturally from its classical expression. For all of the simple one-dimensional systems we will consider here, the Hamiltonian operator is

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{x}),$$

where V is the classical potential.

To show how the Heisenberg equation works, we will solve the harmonic oscillator. Classically, the solution to the harmonic oscillator with potential $V(x) = \frac{1}{2}kx^2$ is sinusoidal motion with frequency $\omega = \sqrt{k/m}$. We will use this observation to write the Hamiltonian as

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2.$$

Now that we have a Hamiltonian, we can immediately write equations of motion for the operators. They are

$$\begin{aligned}\frac{d\hat{x}}{dt} &= -\frac{i}{\hbar}[\hat{x}, \hat{\mathcal{H}}] = -\frac{i}{2m\hbar}[\hat{x}, \hat{p}^2] = \frac{\hat{p}}{m},\\ \frac{d\hat{p}}{dt} &= -\frac{i}{\hbar}[\hat{p}, \hat{\mathcal{H}}] = -\frac{im\omega^2}{2\hbar}[\hat{p}, \hat{x}^2] = -m\omega^2\hat{x}.\end{aligned}$$

These should look familiar: they are nothing more than the classical equations of motion, disguised in hats.

In fact, they are so familiar that we can solve them. We should be very careful, because these are differential equations of operators, not of numbers. Nonetheless, the solution is immediate once we differentiate each equation:

$$\begin{aligned}\frac{d^2\hat{x}}{dt^2} &= \frac{1}{m}\frac{d\hat{p}}{dt} = -\omega^2\hat{x},\\ \frac{d^2\hat{p}}{dt^2} &= -m\omega^2\frac{d\hat{x}}{dt} = -\omega^2\hat{p}.\end{aligned}$$

This implies that each operator oscillates with frequency ω. Fixing boundary conditions, we have

$$\begin{aligned}\hat{x}(t) &= \hat{x}(0)\cos\omega t + \frac{1}{m\omega}\hat{p}(0)\sin\omega t,\\ \hat{p}(t) &= \hat{p}(0)\cos\omega t - m\omega\hat{x}(0)\sin\omega t.\end{aligned}$$

This has one immediate and reassuring consequence: the system is periodic with period $t = \frac{2\pi}{\omega}$. Additionally, you can verify for yourself that the Hamiltonian is invariant, with $\hat{H}(t) = \hat{H}(0)$. This is all expected, and it is good that it happens, but what about the actual system? Is it oscillating like the corresponding classical system would? Equations of operators aren't very useful for answering these physical questions.

One approach we could take is to understand how the expected values of position and momentum change in time. Let the system be in state $|\psi\rangle$; in the Heisenberg picture, all the evolution is contained in the operators, so $\frac{d}{dt}|\psi\rangle = 0$. Let $X(t) = \langle\psi|\hat{x}(t)|\psi\rangle$ and $P(t) = \langle\psi|P(t)|\psi\rangle$ be the expected values of position and momentum. then we have

$$\begin{aligned}\frac{dX}{dt} &= \left\langle\psi\middle|\frac{d\hat{x}}{dt}\middle|\psi\right\rangle = \frac{P(t)}{m},\\ \frac{dP}{dt} &= \left\langle\psi\middle|\frac{d\hat{p}}{dt}\middle|\psi\right\rangle = -m\omega^2X(t).\end{aligned}$$

These are the classical equations of motion, and so the expectations behave exactly like the classical harmonic oscillator.

All of this is both reassuring and boring. If everything about the quantum harmonic oscillator is just like the classical one, then we have come a long way for a little. However, we already know that there must be differences. In the classical harmonic oscillator, the mass can rest at the origin with $x = p = 0$. The uncertainty principle precludes this possibility in the quantum case. Since the Hamiltonian is positive semidefinite (it is a sum of two squares), and the uncertainty principle prohibits $\hat{\mathcal{H}} |\psi\rangle = 0$, the minimum eigenvalue of $\hat{H}$ must be strictly positive.

We can determine what this eigenvalue is by coming at the problem from another angle. Since $\hat{\mathcal{H}}$ is Hermitian, its eigenvectors form a basis. We will label these eigenvectors by $|n\rangle$, where $\hat{\mathcal{H}} |n\rangle = E_n |n\rangle$. Keep in mind that there could in principle be degeneracy in this basis (though it turns out that, in the one-dimensional case, there is not).

We have two different means at our disposal for determining the matrix elements of $\hat{x}(t)$ and $\hat{p}(t)$ in the energy basis. We could use our solutions for the time evolution of the operators to express the matrix elements in terms of their values at $t = 0$:

$$\begin{aligned}
\langle m|\hat{x}(t)|n\rangle &= \langle m|\hat{x}(0)|n\rangle \cos\omega t + \frac{1}{m\omega} \langle m|\hat{p}(0)|n\rangle \sin\omega t, \\
\langle m|\hat{p}(t)|n\rangle &= \langle m|\hat{p}(0)|n\rangle \cos\omega t - m\omega \langle m|\hat{x}(0)|n\rangle \sin\omega t.
\end{aligned}$$

Alternatively, we can use the formal solution to the Heisenberg equation to write

$$\begin{aligned}
\langle m|\hat{x}(t)|n\rangle &= \left\langle m \left| e^{i\hat{\mathcal{H}}t/\hbar} \hat{x}(0) e^{-i\hat{\mathcal{H}}t/\hbar} \right| n \right\rangle = e^{i(E_m - E_n)t/\hbar} \langle m|\hat{x}(0)|n\rangle , \\
\langle m|\hat{p}(t)|n\rangle &= \left\langle m \left| e^{i\hat{\mathcal{H}}t/\hbar} \hat{p}(0) e^{-i\hat{\mathcal{H}}t/\hbar} \right| n \right\rangle = e^{i(E_m - E_n)t/\hbar} \langle m|\hat{p}(0)|n\rangle .
\end{aligned}$$

These expressions look very different, but they must exactly equal. This will give us strong constraints on the matrix elements. If we rewrite $\cos\omega t$ and $\sin\omega t$ as exponentials, the first set of equations become

$$\begin{aligned}
\langle m|\hat{x}(t)|n\rangle &= \frac{1}{2} e^{i\omega t} \left\langle m \left| \hat{x}(0) - \frac{i}{m\omega} \hat{p}(0) \right| n \right\rangle + \frac{1}{2} e^{-i\omega t} \left\langle m \left| \hat{x}(0) + \frac{i}{m\omega} \hat{p}(0) \right| n \right\rangle \\
&\equiv \sqrt{\frac{\hbar}{2m\omega}} \left(e^{i\omega t} \langle m|\hat{a}^\dagger|n\rangle + e^{-i\omega t} \langle m|\hat{a}|n\rangle \right), \\
\langle m|\hat{p}(t)|n\rangle &= \frac{1}{2} e^{i\omega t} \langle m|\hat{p}(0) + im\omega\hat{x}(0)|n\rangle + \frac{1}{2} e^{-i\omega t} \langle m|\hat{p}(0) - im\omega\hat{x}(0)|n\rangle \\
&\equiv i\sqrt{\frac{\hbar m\omega}{2}} \left(e^{i\omega t} \langle m|\hat{a}^\dagger|n\rangle - e^{-i\omega t} \langle m|\hat{a}|n\rangle \right),
\end{aligned}$$

where we have defined the dimensionless operator $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x}(0) + \frac{i}{m\omega} \hat{p}(0) \right)$ for convenience. It is clear from this that, if the matrix elements are nonzero, then $E_m - E_n = \pm\hbar\omega$. The two cases

correspond to different constraints on the matrix elements of $\hat{a}$:

$$E_m = E_n + \hbar\omega: \qquad \begin{cases} \langle m|\hat{a}^\dagger|n\rangle = \sqrt{\frac{2m\omega}{\hbar}}\,\langle m|\hat{x}(0)|n\rangle \\ \langle m|\hat{a}|n\rangle = 0 \end{cases}$$

$$E_m = E_n - \hbar\omega: \qquad \begin{cases} \langle m|\hat{a}^\dagger|n\rangle = 0 \\ \langle m|\hat{a}|n\rangle = \sqrt{\frac{2m\omega}{\hbar}}\,\langle m|\hat{x}(0)|n\rangle \end{cases}$$

The second case is very interesting. It says that $\hat{a}\,|n\rangle$ has a nonzero inner product with a state that has $E_m = E_n - \hbar\omega$, so acting with $\hat{a}$ (and possibly projecting out $|m\rangle$) gives us a way to lower the energy by $\hbar\omega$. But we have already established that the eigenvalue of $\hat{\mathcal{H}}$, which is the energy, must be strictly greater than zero. Therefore, at some point our procedure of lowering with $\hat{a}$ must fail. This happens only when $\hat{a}\,|n\rangle = 0$, in which case the above argument fails.

This is an equation we can solve. In terms of wavefunctions, we have

$$\hat{a}\,|\psi\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)|\psi\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(x\psi(x) + \frac{\hbar}{m\omega}\psi'(x)\right).$$

If this is zero, then we have

$$\psi(x) = A\exp\left(-\frac{m\omega}{2\hbar}x^2\right),$$

where $A = \sqrt[4]{\frac{m\omega}{\pi\hbar}}$ is a normalization constant.

We have found a unique state for which $\hat{a}\,|\psi\rangle = 0$; we label this state $|0\rangle$, and its wavefunction by $\psi_0(x)$. Acting with $\hat{\mathcal{H}}$, we have

$$\begin{aligned}\hat{\mathcal{H}}\,|0\rangle &= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2\right)\psi(x) \\ &= \frac{1}{2}\hbar\omega\psi(x).\end{aligned}$$

Thus, the minimum energy for the quantum harmonic oscillator is $\frac{1}{2}\hbar\omega$. The state $|0\rangle$ is the only state for which acting with $\hat{a}$ does not produce a state with lower energy. But we know that we cannot lower the energy forever, so every energy eigenstate must satisfy $\hat{a}^n\,|\psi\rangle \propto |0\rangle$ for some n. We use this value of n to label the state, so $\hat{a}^n\,|n\rangle \propto |0\rangle$. If we could invert $\hat{a}$, we could use this relation to determine $|n\rangle$. In fact, we can do essentially this; the equations above show that $\hat{a}^\dagger$ raises the energy, so it is a decent candidate for the inverse. The product of $\hat{a}$ and its conjugate is

$$\hat{a}^\dagger\hat{a} = \frac{m\omega}{2\hbar}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right) = \frac{1}{\hbar\omega}\left(\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{\hbar\omega}{2}\right).$$

We recognize the Hamiltonian appearing here, so we have

$$\hat{\mathcal{H}} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).$$

Since $\hat{a}^\dagger$ raises the energy by $\hbar\omega$, the allowed energy values are $\left(n + \frac{1}{2}\right)\hbar\omega$. Comparing this with the Hamiltonian, the operator $\hat{a}^\dagger\hat{a}$ must have the property

$$\hat{a}^\dagger\hat{a}\,|n\rangle = n\,|n\rangle.$$

We call this the number operator. This relation shows that, up to a factor of n, $\hat{a}^\dagger$ is the inverse of $\hat{a}$. So, we should have

$$|n+1\rangle = \alpha_n \hat{a}^\dagger |n\rangle .$$

To fix the normalization α_n, we require

$$1 = \langle n+1|n+1\rangle = \alpha_n^2 \langle n|\hat{a}\hat{a}^\dagger|n\rangle .$$

Since

$$[\hat{a}, \hat{a}^\dagger] = \frac{m\omega}{2\hbar}\left(-\frac{i}{m\omega}[\hat{x},\hat{p}] + \frac{i}{m\omega}[\hat{p},\hat{x}]\right) = 1,$$

we have $\langle n|\hat{a}\hat{a}^\dagger|n\rangle = \langle n|(\hat{a}^\dagger\hat{a}+1)|n\rangle = n+1$. Therefore, $\alpha_n = \frac{1}{\sqrt{n+1}}$. It follows that

$$|n\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n |0\rangle .$$

Let us collect our results. The Hamiltonian $\hat{\mathcal{H}}$ has a spectrum of eigenvectors $|n\rangle$, with eigenvalues $\hbar\omega\left(n+\frac{1}{2}\right)$. The operators

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}(0) + \frac{i}{m\omega}\hat{p}(0)\right), \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}(0) - \frac{i}{m\omega}\hat{p}(0)\right)$$

are called lowering and raising operators respectively, since they have the properties

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle , \qquad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle .$$

The ground state $|0\rangle$ satisfies $\hat{a}\,|0\rangle = 0$.

Example 5.1. Show that every energy eigenstate of the harmonic oscillator satisfies the uncertainty principle at $t = 0$.

Solution: One approach would be to use the position-space representation of $\hat{a}^\dagger$ and act on the ground state wavefunction $\psi_0(x)$ to construct the higher energy wavefunctions, and then determine Δx and Δp by integrating. This would be extremely tedious. Instead, we will take an algebraic approach. We have

$$\hat{x}(0) = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a} + \hat{a}^\dagger\right),$$
$$\hat{p}(0) = -i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a} - \hat{a}^\dagger\right).$$

Therefore,

$$\langle n|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle n|(\hat{a}+\hat{a}^\dagger)|n\rangle = 0,$$
$$\langle n|\hat{p}|n\rangle = -i\sqrt{\frac{\hbar m\omega}{2}}\,\langle n|(\hat{a}-\hat{a}^\dagger)|n\rangle = 0.$$

The variances are

$$\begin{aligned}
\langle n|\hat{x}^2|n\rangle &= \frac{\hbar}{2m\omega}\langle n|(\hat{a}+\hat{a}^\dagger)^2|n\rangle \\
&= \frac{\hbar}{2m\omega}\langle n|(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})|n\rangle \\
&= \frac{\hbar}{m\omega}\left(n+\frac{1}{2}\right) \\
\langle n|\hat{p}^2|n\rangle &= -\frac{\hbar m\omega}{2}\langle n|(\hat{a}-\hat{a}^\dagger)^2|n\rangle \\
&= \frac{\hbar m\omega}{2}\langle n|(\hat{a}\hat{a}^\dagger+\hat{a}^\dagger\hat{a})|n\rangle \\
&= \hbar m\omega\left(n+\frac{1}{2}\right).
\end{aligned}$$

Therefore,

$$\Delta x\Delta p = \hbar\left(n+\frac{1}{2}\right) \geq \frac{\hbar}{2}.$$

Note that the inequality is saturated at $n = 0$. Indeed, we have already shown that the ground state wavefunction is Gaussian, and we showed in Example 4.2 that Gaussian wavefunctions saturate the uncertainty relation.

Since we have an explicit construction for the energy eigenstates, we can expand any state $|\psi\rangle$ in this basis, as

$$|\psi\rangle = \sum_{n=0}^{\infty}\psi_n|n\rangle.$$

We can also write the operators $\hat{x}(t)$ and $\hat{p}(t)$ in the energy basis, using the expression in terms of raising and lowering operators:

$$\begin{aligned}
\langle n'|\hat{x}(t)|n\rangle &= e^{i(E_{n'}-E_n)t/\hbar}\langle n'|\hat{x}(0)|n\rangle \\
&= e^{i(n'-n)\omega t}\sqrt{\frac{\hbar}{2m\omega}}\langle n'|(\hat{a}+\hat{a}^\dagger)|n\rangle \\
&= e^{i(n'-n)\omega t}\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n'}\delta_{n',n+1}+\sqrt{n}\delta_{n'+1,n}), \\
\langle n'|\hat{p}(t)|n\rangle &= e^{i(E_{n'}-E_n)t/\hbar}\langle n'|\hat{p}(0)|n\rangle \\
&= -ie^{i(n'-n)\omega t}\sqrt{\frac{\hbar m\omega}{2}}\langle n'|(\hat{a}-\hat{a}^\dagger)|n\rangle \\
&= -ie^{i(n'-n)\omega t}\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n'}\delta_{n',n+1}-\sqrt{n}\delta_{n'+1,n}).
\end{aligned}$$

With these expressions, we can determine any quantities of interest as a function of time for any

state. For example, the expected value of position is

$$\begin{aligned}\langle\psi|\hat{x}(t)|\psi\rangle &= \sum_{n,n'=0}^{\infty} \langle\psi|n'\rangle \langle n'|\hat{x}(t)|n\rangle \langle n|\psi\rangle \\ &= \sqrt{\frac{\hbar}{2m\omega}} \sum_{n,n'=0}^{\infty} \psi_n \psi_{n'}^* e^{i(n'-n)\omega t}(\sqrt{n'}\delta_{n',n+1} + \sqrt{n}\delta_{n'+1,n}) \\ &= \sqrt{\frac{2\hbar}{m\omega}} \left[\cos(\omega t) \sum_{n=0}^{\infty} \left(\sqrt{n+1}\,\mathrm{Re}(\psi_n \psi_{n+1}^*)\right) - \sin(\omega t) \sum_{n=0}^{\infty} \left(\sqrt{n+1}\,\mathrm{Im}(\psi_n^* \psi_{n+1})\right)\right].\end{aligned}$$

The two sums in the final equation, though complicated, are just numbers depending on $|\psi\rangle$.

Knowing the energy eigenbasis thus constitutes a solution to the dynamic problem. In the Schrödinger picture, we will capitalize on this idea to develop a much more systematic way of solving for the dynamics of a system.

Example 5.2. Show that the Hamiltonian is invariant by determining the time evolution of the raising and lowering operators.

Solution: Using the Heisenberg equation, we have

$$\frac{d\hat{a}}{dt} = -\frac{i}{\hbar}[\hat{\mathcal{H}}, \hat{a}] = -\frac{i}{\hbar}\sqrt{\frac{m\omega}{2\hbar}} \left[\frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2, \hat{x} + \frac{i}{m\omega}\hat{p}\right].$$

Evaluating the commutator, we obtain

$$\frac{d\hat{a}}{dt} = -\frac{i}{\hbar}\sqrt{\frac{m\omega}{2\hbar}} \left(\frac{-i\hbar}{m}\hat{p} - \hbar\omega\hat{x}\right) = i\omega\hat{a},$$

so $\hat{a}(t) = e^{i\omega t}\hat{a}(0)$. Thus,

$$\hat{H}(t) = \hbar\omega\left(\hat{a}^\dagger(t)\hat{a}(t) + \frac{1}{2}\right) = \hbar\omega\left(\hat{a}^\dagger(0)\hat{a}(0) + \frac{1}{2}\right) = \hat{H}(0).$$

5.2 Schrödinger Picture

In the Heisenberg picture, operators evolve in time while states remain fixed. In the Schrödinger picture, we reverse this, and leave operators fixed while letting states evolve. To see how this can work, look carefully at the matrix element of an operator. Using the formal solution to the Heisenberg equation, we have

$$\langle\phi|\hat{A}(t)|\psi\rangle = \left\langle \phi \,\middle|\, e^{i\hat{H}t/\hbar}\hat{A}(0)e^{-i\hat{H}t/\hbar} \,\middle|\, \psi \right\rangle.$$

In the Heisenberg picture, we thought of this as a changing operator sandwiched between fixed states. However, we could also choose to look at it as the fixed operator $\hat{A}(0)$ sandwiched between evolving states $|\phi(t)\rangle = e^{-i\hat{H}t/\hbar}|\phi(0)\rangle$ and $|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|\psi(0)\rangle$.

If states evolve in this way, then they satisfy the differential equation

$$i\hbar \frac{d\,|\psi\rangle}{dt} = \hat{\mathcal{H}}\,|\psi\rangle\,.$$

This is Schrödinger's equation. It is much easier to work with than Heisenberg's equation. In fact, we can easily write down its solution. If we expand the initial state in terms of energy eigenstates as

$$|\psi(0)\rangle = \sum_n \psi_n\,|n\rangle\,,$$

then it is clear that

$$|\psi(t)\rangle = \sum_n \psi_n e^{-iE_n t/\hbar}\,|n\rangle\,.$$

Therefore, as long as we have the eigenstates $|n\rangle$, the system is essentially solved. The bulk of solving Schrödinger's equation is determining the eigenstates of $\hat{\mathcal{H}}$. For this reason, the eigenvalue equation

$$\hat{\mathcal{H}}\,|\psi\rangle = E\,|\psi\rangle$$

is sometimes called the time-independent Schrödinger equation.

Example 5.3. Solve the free-particle Hamiltonian $\hat{H} = \frac{\hat{p}^2}{2m}$ by determining its eigenstates. Use this to determine the time evolution of a Gaussian wavepacket

$$\psi(x, t=0) = \frac{1}{(2\pi)^{1/4}\sigma^{1/2}} e^{-x^2/4\sigma^2}.$$

Solution: The eigenvectors of $\hat{\mathcal{H}}$ are the same as the eigenvectors of $\hat{k}$, so the energy eigenstates are simply $|k\rangle$. Thus, to solve for the evolution of $\psi(x)$, we need to write it in the wavenumber basis. We find

$$\tilde{\psi}(k, t=0) = \langle k|\psi(0)\rangle = \frac{1}{(2\pi)^{3/4}\sigma^{1/2}} \int_{-\infty}^{\infty} dx\, e^{-ikx} e^{-x^2/4\sigma^2} = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma} e^{-\sigma^2 k^2}.$$

The energy of $|k\rangle$ is $\frac{\hbar^2 k^2}{2m}$, so it is multiplied by the factor $e^{-i\hbar k^2 t/2m}$. Therefore,

$$\tilde{\psi}(k, t) = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\sigma} \exp\left[-\left(\sigma^2 + \frac{i\hbar t}{2m}\right) k^2\right].$$

In position space, this is

$$\begin{aligned}\psi(x, t) &= \frac{\sqrt{\sigma}}{2^{1/4}\pi^{3/4}} \int_{-\infty}^{\infty} dk\, e^{ikx} e^{-(\sigma^2 + i\hbar t/2m)k^2} \\ &= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\sigma}{A}} e^{-x^2/4A},\end{aligned}$$

where $A = \sigma^2 + \frac{i\hbar t}{2m}$. Since $|A|$ is increasing in time, the wavefunction spreads out.

We solved the harmonic oscillator in the Heisenberg picture, but the method was exploratory and ad hoc. In the Schrödinger picture, it is clear from the outset what the goal is: determine the eigenstates of the harmonic oscillator Hamiltonian. We can use the raising and lowering operators we found to expedite this process. The Hamiltonian is

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).$$

The commutator of the raising and lowering operators is $[\hat{a}, \hat{a}^\dagger] = 1$, which means

$$[\hat{a}, \hat{\mathcal{H}}] = \hbar\omega\hat{a}, \qquad [\hat{a}^\dagger, \hat{\mathcal{H}}] = -\hbar\omega\hat{a}]^\dagger.$$

Thus, if $\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle$, then

$$\hat{\mathcal{H}}(\hat{a}\left|\psi\right\rangle) = (\hat{a}\hat{\mathcal{H}} - [\hat{a}, \hat{\mathcal{H}}])\left|\psi\right\rangle = (E - \hbar\omega)\hat{a}\left|\psi\right\rangle.$$

Thus, if $\hat{a}\left|\psi\right\rangle \neq 0$, it is an energy eigenstate with energy $E - \hbar\omega$. Since the Hamiltonian is positive semidefinite, we cannot lower the energy forever, so the lowest energy state $\left|0\right\rangle$ must satisfy $\hat{a}\left|0\right\rangle = 0$.

Similarly, $\hat{a}^\dagger\left|\psi\right\rangle$ is a state with energy $E + \hbar\omega$, so the nth state $\left|n\right\rangle$ is proportional to $(\hat{a}^\dagger)\left|0\right\rangle$. We showed in the last section that the exact relation is

$$\left|n\right\rangle = \frac{1}{\sqrt{n!}}(\hat{a}^\dagger)^n\left|0\right\rangle.$$

In the Heisenberg picture, since $\hat{x}$ varied with time, it was not obvious how to write a wavefunction. In the Schrödinger picture $\hat{x}$ is fixed, so $\psi(x) = \langle x|\psi\rangle$ is well-defined for all time. For the energy eigenstates, only the initial wavefunction is important, since

$$\psi_n(x,t) = \langle x|n(t)\rangle = e^{-i\omega(n+1/2)t}\psi_n(x,0).$$

We showed in the previous section that

$$\psi_0(x) = \sqrt[4]{\frac{m\omega}{\pi\hbar}}\exp\left(-\frac{m\omega}{2\hbar}x^2\right).$$

Therefore,

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(\frac{m\omega}{2\hbar}\right)^{n/2}\left(x - \frac{\hbar}{m\omega}\frac{d}{dx}\right)^n\psi_0(x).$$

We can simplify these relations by defining a characteristic length $x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$ and the dimensionless variable $y \equiv x/x_0$. Then

$$\psi_0(y) = \pi^{-1/4}x_0^{-1/2}\exp\left(-y^2/2\right),$$
$$\psi_n(y) = \frac{2^{-n/2}}{\sqrt{n!}}\left(y - \frac{d}{dy}\right)^n\psi_0(y).$$

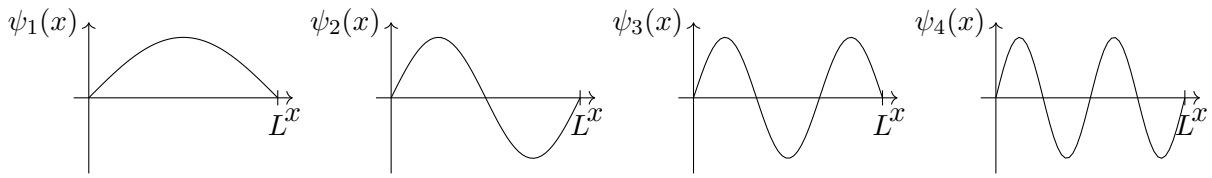


Figure 3: The eigenstates of the infinite well Hamiltonian.

Using these relations, we can write the first few eigenstates:

$$\psi_1(x) = \frac{\sqrt{2}}{\pi^{1/4} x_0^{1/2}} y e^{-y^2/2},$$
$$\psi_2(x) = \frac{1}{\pi^{1/4} x_0^{1/2}} (2y^2 - 1) e^{-y^2/2}.$$

It is easy to see that the pattern of a polynomial in y multiplied by the Gaussian factor will continue. The polynomials which appear are called the Hermite polynomials.

Another interesting potential we can solve is the infinite well, also known as the particle in a box. The potential is

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq L, \\ \infty & \text{otherwise} \end{cases}.$$

We can solve the time-independent Schrödinger equation in position space. The potential is, in effect, a boundary condition: the wavefunction must vanish outside of the interval $[0, L]$. Continuity forces $\psi(0) = \psi(L) = 0$. Thus, we are seeking solutions to

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi(x)$$

which satisfy these conditions. We know that the eigenstates of the free particle Hamiltonian are $|k\rangle$, so we are looking for wavefunctions $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{-ikx}$ that satisfy the boundary conditions. Unfortunately, none of them do, since $|\psi_k(x)| = (2\pi)^{-1/2}$ everywhere.

To fix this, we remember that the energy eigenvalue of $|k\rangle$ is $\frac{\hbar^2 k^2}{2m}$, so there is a twofold degeneracy. Thus, a linear combination of $|k\rangle$ and $|-k\rangle$ is also an energy eigenstate. Since $\psi_k(0) = \psi_{-k}(0)$, we must subtract the two functions in order to satisfy the boundary condition at 0, which gives $\psi(x) \propto \sin(kx)$. Then we must also have $\psi(L) = 0$, which implies $kL = n\pi$. Therefore, the eigenstates of the infinite well are

$$\psi_n(x) = \begin{cases} \sqrt{2/L} \sin\left(\frac{n\pi x}{L}\right) & \text{if } 0 \leq x \leq L \\ 0 & \text{otherwise} \end{cases}.$$

The constant $\sqrt{2/L}$ is obtained by normalizing the wavefunction. These wavefunctions are shown in Figure 3.

The energies of these states are $E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2mL^2} n^2$. The ground state energy E_1 increases as L^{-2} as the space occupied by the particle shrinks. This is a phenomenon known as confinement

energy, and it can be explained in terms of the uncertainty principle. As $L \to 0$, the uncertainty in momentum grows as roughly $\Delta p \sim \hbar/L$, so the energy is on the order of $\frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2mL^2}$. Indeed, up to a factor of π^2, this is exactly what we found.

Example 5.4. Assume the particle is initially distributed uniformly throughout the well, with $\psi(x,0) = L^{-1/2}$ inside the well (and zero outside). Determine $\psi(x,t)$.

Solution: We have already determined the energy eigenstates, so we only need to express $|\psi\rangle$ in terms of them. We have

$$\langle n|\psi\rangle = \frac{\sqrt{2}}{L}\int_0^L dx\, \sin\frac{n\pi x}{L} = \frac{\sqrt{2}}{n\pi}(1-\cos(n\pi)).$$

Therefore,

$$|\psi(0)\rangle = \frac{2\sqrt{2}}{\pi}\sum_{j=0}^{\infty}\frac{|2j+1\rangle}{2j+1}.$$

The energy of $|2j+1\rangle$ is $\frac{\hbar^2\pi^2}{2mL^2}(2j+1)^2$, so

$$|\psi(t)\rangle = \frac{2\sqrt{2}}{\pi}\sum_{j=0}^{\infty}\exp\left(\frac{i\hbar\pi^2(2j+1)^2}{2mL^2}t\right)\frac{|2j+1\rangle}{2j+1}.$$

Therefore,

$$\psi(x,t) = \frac{4}{\pi\sqrt{L}}\sum_{j=0}^{\infty}\exp\left(\frac{i\hbar\pi^2(2j+1)^2}{2mL^2}t\right)\frac{\sin((2j+1)\pi x/L)}{2j+1}$$

A more difficult, but also more interesting, case is the finite well, with potential

$$V(x) = \begin{cases} -V_0 & \text{if } -L/2 \le x \le L/2 \\ 0 & \text{otherwise} \end{cases}.$$

There are three regions, $x < -L/2$, $-L/2 \le x \le L/2$, and $x > L/2$. We label these I, II, and III, respectively. The Schrödinger equation in regions I and III is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi,$$

and the equation in region II is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E+V_0)\psi.$$

We will focus here on the case where $E < 0$. Remember that, classically, this is the condition for the particle to be bound to the well.

In regions I and III, the solutions are

$$\psi_I(x) = Ae^{\kappa x},$$
$$\psi_{III}(x) = De^{-\kappa x},$$

where $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$. Note that, since $E < 0$, κ is real. In each region, both exponentials solve the equation, but we have kept only the solutions which decay to zero at infinity.

In region II, the solution is

$$\psi_{II}(x) = Be^{ikx} + Ce^{-ikx},$$

where $k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$.

Since the potential is finite everywhere, both $\psi(x)$ and $\psi'(x)$ must be continuous. Continuity of $\psi(x)$ gives the conditions

$$Ae^{-\kappa L/2} = Be^{-ikL/2} + Ce^{ikL/2}, \qquad De^{-\kappa L/2} = Be^{ikL/2} + Ce^{-ikL/2}.$$

Continuity of $\psi'(x)$ requires that

$$\kappa Ae^{-\kappa L/2} = ikBe^{-ikL/2} - ikCe^{ikL/2}, \qquad -\kappa De^{-\kappa L/2} = ikBe^{ikL/2} - ikCe^{-ikL/2}.$$

Dividing each pair of equations gives

$$\frac{A}{D} = \frac{Be^{-ikL/2} + Ce^{ikL/2}}{Be^{ikL/2} + Ce^{-ikL/2}} = \frac{-Be^{-ikL/2} + Ce^{ikL/2}}{Be^{ikL/2} - Ce^{-ikL/2}}.$$

This can be solved in two ways: either $B = C$ and $A = D$ (the symmetric case), or $B = -C$ and $A = -D$ (the antisymmetric case).

In the symmetric case, the equations reduce to

$$Ae^{-\kappa L/2} = 2B\cos(kL/2), \qquad \kappa Ae^{-\kappa L/2} = 2kB\sin(kL/2).$$

Dividing these gives $\kappa = k\tan(kL/2)$. In the antisymmetric case, we similarly have

$$Ae^{-\kappa L/2} = -2iB\sin(kL/2), \qquad \kappa Ae^{-\kappa L/2} = 2ikB\cos(kL/2),$$

so $\kappa = -k\cot(kL/2)$. Since κ and k both depend on the energy, these are transcendental equations in the energy which must be satisfied by any bound state. We thus find a discrete spectrum of bound states. There are only a finite number of bound states, as opposed to the infinite well where there were infinitely many bound states.

Schematically, the wavefunctions for these states look like smoothed out versions of the eigenstates of the infinite well. Instead of the wavefunction suddenly being clamped to zero outside the well, it exponentially decays starting at the walls of the well. An example is shown in Figure 4.

5.3 Symmetries and Conserved Quantities

In Section 1, we showed how a continuous symmetry in the Lagrangian generates a conserved quantity via Noether's theorem. We also showed that this conserved quantity generates the same symmetry through the Poisson bracket. This is a powerful organizing principle, and exposes a much deeper structure to classical mechanics than a Newtonian formulation would suggest.

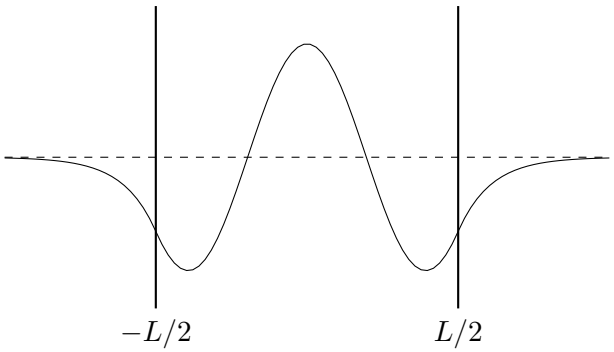


Figure 4: An energy eigenstate of the finite well, with an oscillating solution smoothly connecting to an exponential decay.

The same connection exists in quantum mechanics; in fact, the link between symmetries and conserved quantities runs even deeper in the quantum setting. We saw in Section 3.3 that symmetries are implemented by operators. Observables are also operators, so the notion of a symmetry generating a conserved quantity can be made very precise. Indeed, there is a sense in which symmetries *are* conserved quantities. The mathematical underpinnings of this connection are given here, for those interested.

Mathematical aside: In Section 2, we developed the notion of a group, one of the simplest algebraic structures. The operators on a given Hilbert space $\mathcal{H}$ form an abelian group under addition, but clearly they have far more structure. For one, we can multiply operators by scalars in $\mathbb{C}$; this gives them the structure of a vector space. Additionally, operators can be multiplied together in a way that interacts naturally with the addition and scalar multiplication. This gives the set of operators the structure of an *algebra*; very roughly, an algebra is a vector space where the vectors can be multiplied.

In quantum mechanics, we deal with *bounded* operators. An operator $\hat{A}$ is bounded if it has the property

$$\sup_{|\psi\rangle \in \mathcal{H}} \frac{|\,\langle\psi|\hat{A}|\psi\rangle\,|}{\langle\psi|\psi\rangle} < \infty.$$

We denote the algebra of bounded operators on a Hilbert space $\mathcal{H}$ by $\mathcal{B}(\mathcal{H})$.

An endomorphism of an algebraic structure is a homomorphism from that structure to itself (and recall that a homomorphism is a map which respects the structure of its domain). An automorphism is a bijective homomorphism. Automorphisms are symmetries. For example, in the context of groups, the map $\phi : G \to G$ given by $a \mapsto gag^{-1}$ for some fixed $g \in G$ is an automorphism. To see this, we verify that it is a homomorphism:

$$\phi(ab) = gabg^{-1} = gag^{-1}gbg^{-1} = \phi(a)\phi(b),$$

and that it is bijective, which you can verify for yourself. An automorphism constructed in this manner is called an inner automorphism. An inner automorphism is specified by the element g.

The algebra $\mathcal{B}(\mathcal{H})$ has a special property: all automorphisms are inner. This means that every symmetry is built from an operator in $\mathcal{B}(\mathcal{H})$. In physical terms, every symmetry of the space of observables has a corresponding observable.

We will start by considering the simplest example from classical mechanics, the momentum of a free particle. Using Heisenberg's equation, we can show that it is conserved:

$$\frac{d\hat{p}}{dt} = -\frac{i}{\hbar}[\hat{p}, \hat{\mathcal{H}}] = 0,$$

since $\mathcal{H} = \hat{p}^2/2m$. We also know that momentum generates a translation operator, via

$$\hat{T}(a) = e^{-i\hat{p}a/\hbar}.$$

Translation is a symmetry of the free particle Hamiltonian, since

$$\hat{T}(a)\hat{\mathcal{H}}\hat{T}(a)^{-1} = e^{-i\hat{p}a/\hbar}\frac{\hat{p}^2}{2m}e^{i\hat{p}a/\hbar} = \hat{\mathcal{H}}.$$

What is the connection between these facts? From our classical intuition, we expect that somehow the symmetry in the Hamiltonian (which is equivalent, by duality, to a symmetry in the Lagrangian) generates the conserved quantity $\hat{p}$. Indeed, this is the case. Differentiating the equation of the symmetry, we have

$$0 = \frac{d\hat{\mathcal{H}}}{da} = \frac{d}{da}\left(\hat{T}(a)\hat{\mathcal{H}}\hat{T}(a)^{-1}\right) = -\frac{i}{\hbar}(\hat{p}\hat{\mathcal{H}} - \hat{\mathcal{H}}\hat{p}) = -\frac{i}{\hbar}[\hat{p}, \hat{\mathcal{H}}] = \frac{d\hat{p}}{dt}.$$

This equations works just as well when read from right to left. Given that $\hat{p}$ does not change in time, we can establish that the symmetry operator it generates is in fact a symmetry of the Hamiltonian.

We can easily generalize this argument. Let $\hat{S}(\phi)$ be a one-parameter family of unitary operators, with $\hat{S}(\phi)^\dagger = \hat{S}(-\phi)$. Moreover, assume $\hat{S}(\phi)$ is a symmetry of the Hamiltonian, so that

$$\hat{S}(\phi)\hat{\mathcal{H}}\hat{S}(\phi)^{-1} = \hat{\mathcal{H}}.$$

Since $\hat{S}(\phi)$ is unitary, we have $\hat{S}(\phi)^{-1} = \hat{S}(\phi)^\dagger = \hat{S}(-\phi)$. Then, differentiating with respect to ϕ, we find

$$\frac{d\hat{S}}{d\phi}\hat{\mathcal{H}}\hat{S}(-\phi) - \hat{S}(\phi)\hat{\mathcal{H}}\frac{d\hat{S}}{d\phi} = 0.$$

Using the fact that $\hat{S}(\phi)$ is a symmetry of the Hamiltonian, we can write this as

$$-\frac{i}{\hbar}\left[i\hbar\frac{d\hat{S}}{d\phi}\hat{S}(-\phi), \hat{\mathcal{H}}\right] = 0.$$

This gives an explicit formula, $i\hbar\frac{d\hat{S}}{d\phi}\hat{S}(-\phi)$, for the conserved quantity generated by the symmetry $\hat{S}(\phi)$. For example, in the case of the translation operator, we have

$$i\hbar\frac{d\hat{T}}{da}\hat{T}(-a) = \hat{p}e^{-i\hat{p}a/\hbar}e^{i\hat{p}a/\hbar} = \hat{p}.$$

It is even easier to show that a conserved quantity generates a symmetry. Let $\hat{A}$ be conserved, so that

$$\frac{d\hat{A}}{dt} = -\frac{i}{\hbar}[\hat{A}, \hat{\mathcal{H}}] = 0.$$

Then consider the unitary family $\hat{S}(\phi) = e^{-i\hat{A}\phi/\hbar}$. We have

$$\frac{d}{d\phi}\left(\hat{S}(\phi)\hat{\mathcal{H}}\hat{S}(\phi)^{-1}\right) = -\frac{i}{\hbar}\hat{S}(\phi)[\hat{A},\hat{\mathcal{H}}]\hat{S}(\phi)^{-1} = 0.$$

Therefore, $\hat{S}(\phi)$ is a symmetry of the Hamiltonian. We can summarize these results in a theorem.

Theorem 5.1 (Quantum Noether's Theorem)**.** Let $\hat{S}(\phi)$ be a family of unitary operators such that $\hat{S}(\phi)^{-1} = \hat{S}(-\phi)$. Then $\hat{S}(\phi)$ is a symmetry of the Hamiltonian if and only if

$$i\hbar\frac{d\hat{S}}{d\phi}\hat{S}(-\phi)$$

is a constant of motion with respect to the Heisenberg equation.

Example 5.5. Classically, Galilean symmetry led to the conservation of center of mass velocity (cf. Example 1.3). Show that the same relation holds in quantum mechanics, using a system of N particles on a line which interact with each other through a pairwise potential $V(\hat{x}_i - \hat{x}_j)$.

Solution: The Hamiltonian for the system is

$$\hat{\mathcal{H}} = \sum_{i=1}^{N}\frac{\hat{p}_i^2}{2m} + \sum_{i<j}V(\hat{x}_i - \hat{x}_j).$$

The Galilean symmetry changes both position and momentum, according to the recipe

$$x \mapsto x - vt, \qquad p \mapsto p - mv.$$

Thus, the operator should be a product of the normal translation operator and the momentum-translation operator we derived in Example 3.5. Additionally, every particle needs to have its position and momentum translated. Therefore, the operator implementing Galilean symmetry is

$$\hat{S}(v) = \prod_{i=1}^{N} e^{i\hat{p}_i vt/\hbar}\prod_{i=1}^{N} e^{-i\hat{x}mv/\hbar} = \exp\left(\frac{i}{\hbar}v(\hat{P}t - M\hat{X})\right),$$

where $\hat{P}$ is the total momentum, M is the total mass, and $\hat{X}$ is the center of mass position. This is not exactly a symmetry of the Hamiltonian; it changes the Hamiltonian by

$$\hat{S}(v)\hat{\mathcal{H}}\hat{S}(-v) = \hat{H} + \hat{P}v + \frac{1}{2}Mv^2,$$

which you are encouraged to verify for yourself. Differentiating, we have

$$-\frac{i}{\hbar}\left[i\hbar\frac{d\hat{S}}{dv}\hat{S}(-v), \hat{H} + \hat{P}v + \frac{1}{2}Mv^2\right] = \hat{P} + Mv.$$

We can use this to evaluate the time derivative of $i\hbar\frac{d\hat{S}}{dv}\hat{S}(-v) = M\hat{X} - \hat{P}t$. Since

$$-\frac{i}{\hbar}\left[M\hat{X} - \hat{P}t, \hat{P}v + \frac{1}{2}Mv^2\right] = Mv,$$

we have

$$\begin{aligned}\frac{d}{dt}\left(M\hat{X}-\hat{P}t\right) &= -\frac{i}{\hbar}\left[i\hbar\frac{d\hat{S}}{dv}\hat{S}(-v),\hat{\mathcal{H}}\right]+\frac{\partial}{\partial t}\left(M\hat{X}-\hat{P}t\right)\\ &= \hat{P}+Mv-Mv-\hat{P}\\ &= 0.\end{aligned}$$

Therefore, $M\hat{X}-\hat{P}t$ is conserved, meaning the center of mass moves with a constant velocity represented by the operator $\frac{\hat{P}}{M}$.

All of our analysis so far has been in the Heisenberg picture. What does it mean to have a constant of motion in the Schrödinger picture? If we have an operator $\hat{A}$ which commutes with the Hamiltonian, then by Theorem 4.2, there is a basis of simultaneous eigenvectors of $\hat{A}$ and $\hat{\mathcal{H}}$. This means we can choose the energy basis to consist of eigenvectors of $\hat{A}$. Then, if an initial state $|\psi\rangle$ is an eigenvector of $\hat{A}$, it will be for all time, since energy eigenstates are stable under time evolution.

For example, consider the parity operator $\hat{\mathbb{P}}$, which is defined by

$$\hat{\mathbb{P}}\hat{x}=-\hat{x},\qquad \hat{\mathbb{P}}\hat{p}=-\hat{p}.$$

In the position basis, $\hat{\mathbb{P}}$ acts on wavefunctions by $\hat{\mathbb{P}}\psi(x)=\psi(-x)$, so its eigenstates are even and odd wavefunctions. Thus, whenever $[\hat{\mathbb{P}},\hat{\mathcal{H}}]=0$, we can choose the energy eigenstates to all have either even or odd parity. The harmonic oscillator Hamiltonian commutes with parity, since $\hat{\mathbb{P}}\hat{p}^2=\hat{p}^2=\hat{p}^2\hat{\mathbb{P}}$ and $\hat{\mathbb{P}}\hat{x}^2=\hat{x}^2=\hat{x}^2\hat{\mathbb{P}}$. And indeed, in Section 5.2, we computed the first few energy eigenstates and found that they alternated between even and odd functions.

Note that parity is not a continuous symmetry. We have thus gone beyond the classical Noether theorem by showing that states with definite parity have that parity conserved when the Hamiltonian commutes with $\hat{\mathbb{P}}$. Moreover, in this case there is no distinction between the symmetry and the conserved quantity: parity is both the symmetry operator and the conserved observable.

We can do better than just looking at a single symmetry operator, while still keeping symmetries discrete. Noether's theorem told us about continuous groups of symmetries; we can also develop results for finite groups of symmetries. Let G be a group of operators which commute with the Hamiltonian. For example, $G=\{\hat{\mathbb{I}},\hat{\mathbb{P}}\}$ is such a group for the harmonic oscillator (where $\hat{\mathbb{I}}$ is the identity operator). Since $G\simeq\mathbb{Z}_2$, we have a homomorphism $\phi:\mathbb{Z}_2\to G$. Since G is a subgroup of the group of invertible operators on the Hilbert space, we can compose ϕ with an inclusion to obtain a homomorphism from ϕ to this group of operators. This means ϕ is an infinite-dimensional representation of G.

In Section 2.2, we developed the theory of finite-dimensional representations of finite groups. There is actually almost no difficulty in applying this theory here: we simply reduce the infinite-dimensional representation into the finite-dimensional irreducible representations. For example, the $\mathbb{Z}_2$ parity symmetry has two irreps, each one-dimensional:

$\mathbb{Z}_2$	$e\,[1]$	$a\,[1]$
A_1	1	1
A_2	1	-1

This means the Hilbert space splits into one-dimensional invariant subspaces, each of which is either even or odd under parity (corresponding to the representations A_1 and A_2 respectively). Since the group commutes with the Hamiltonian, the invariant subspaces of G are also invariant under the action of the Hamiltonian. A one-dimensional invariant subspace is an eigenvector, so we have shown that the eigenstates of the Hamiltonian split into the two representations of $\mathbb{Z}_2$.

We can apply the same analysis with larger groups. For example, consider a two-dimensional system which is symmetric under rotations by $\phi = 2\pi/N$ (that is, the rotation operator $\hat{R}_z(\phi)$ commutes with the Hamiltonian). This rotation generates the group $\mathbb{Z}_n$, which we know from Section 2.2 to have n one-dimensional representations. The character of the generator $\hat{R}_z(\phi)$ in the nth representation is $e^{in\phi}$, which means every eigenstate has a wavefunction satisfying

$$\psi(r, \theta + \phi) = e^{in\phi}\psi(r, \theta)$$

for some n.

Example 5.6. Consider an electron in a crystal lattice in d dimensions. Assume the lattice is generated by the vectors $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_d$; that is, the atoms are at the positions

$$n_1\boldsymbol{a}_1 + \ldots + n_d\boldsymbol{a}_d,$$

where $n_i \in \mathbb{Z}$. Using the representation theory of $\mathbb{Z}^d$, prove Bloch's theorem, which states that the energy eigenstates are of the form

$$\psi(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}u(\boldsymbol{r}),$$

where the function $u(\boldsymbol{r})$ has the periodicity of the lattice.

Solution: The symmetry group of the lattice is the group of translations $\hat{T}(n_1\boldsymbol{a}_1 + \ldots + n_d\boldsymbol{a}_d)$, which is isomorphic to $\mathbb{Z}^d$. Since $\mathbb{Z}^d$ is Abelian, the representations are all one-dimensional. The characters of $\mathbb{Z}$ are $\chi_k(n) = e^{-2\pi ikn}$, with $k \in [0, 1)$, and so it is relatively easy to see that the characters of $\mathbb{Z}^d$ are

$$\chi_{k_1,\ldots,k_d}(n_1, \ldots, n_d) = e^{-2\pi i(k_1n_1+\ldots+k_dn_d)}.$$

This means that all the eigenstates of the Hamiltonian must satisfy

$$\psi(\boldsymbol{r} + \boldsymbol{a}_i) = e^{-2\pi ik_i}\psi(\boldsymbol{r});$$

these d equations are sufficient to imply the more general relation

$$\psi(\boldsymbol{r} + n_1\boldsymbol{a}_1 + \ldots + n_d\boldsymbol{a}_d) = e^{-2\pi i(n_1k_1+\ldots+n_dk_d)}\psi(\boldsymbol{r}).$$

For any lattice $\boldsymbol{a}_i$, we can construct a reciprocal lattice $\boldsymbol{b}_i$ which has the property $\boldsymbol{a}_i \cdot \boldsymbol{b}_j = 2\pi\delta_{ij}$. Let $\boldsymbol{k} = k_1\boldsymbol{b}_1 + \ldots + k_n\boldsymbol{b}_n$. Then we can write the previous condition as

$$\psi(\boldsymbol{r} + \boldsymbol{a}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{a}}\psi(\boldsymbol{r}),$$

whenever $\boldsymbol{a}$ is a lattice vector. Now define

$$u(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\psi(\boldsymbol{r}).$$

The previous equation implies that $u(\boldsymbol{r}+\boldsymbol{a}) = u(\boldsymbol{r})$. Therefore, every energy eigenstate is of the form

$$\psi(\boldsymbol{r}) = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}u(\boldsymbol{r}),$$

where $u(\boldsymbol{r})$ has the periodicity of the lattice, and this proves Bloch's theorem.

When the symmetry group is non-Abelian, representations can be more than one-dimensional, and so the situation becomes more complicated. For example, assume we have a triangular molecule with identical atoms at each vertex. In Section 2.2, we showed that the representations of $D_3 \simeq S_3$ have the character table

D_3	e [1]	(231) [2]	(12) [3]
A_1	1	1	1
A_2	1	1	-1
E_1	2	-1	0

This means that the eigenstates of the Hamiltonian are one of three types. If they live in the representation A_1, then they are unaffected by any symmetries of the molecule. If they live in A_2, then rotations about the three-fold axis leave the state unaffected, while rotations by π through a two-fold axis negate the state. If two eigenstates live in the representation E_2, then they transform under the two-dimensional representation given in Section 2.2.

The character table of D_3 allows us to determine the possible eigenstates which can form from combinations of the ground states of electrons in each atom. A chemist would say we are determining the molecular orbitals that result from hybridization of s orbitals in the atoms. Let $\psi_i(\boldsymbol{r}) = \psi_0(\boldsymbol{r} - \boldsymbol{r}_i)$ be the ground state wavefunctions, with $i = 1, 2, 3$ labeling the sites. Our space of possible wavefunctions is

$$\left\{ \sum a_i \psi_0(\boldsymbol{r} - \boldsymbol{r}_i) \mid a_i \in \mathbb{C} \right\},$$

so it is isomorphic to $\mathbb{C}^3$. The group D_3 acts on this space in the natural way, by permuting the sites. Since the operators forming D_3 commute with the Hamiltonian, finding energy eigenstates is equivalent to finding invariant subspaces of D_3.

To find these invariant subspaces, we project the representation of D_3 on our three-dimensional space onto the irreps. You can verify for yourself that the characters of this representation are $(3, 0, 1)$, in the order given in the character table above. Therefore, this representation decomposes into $A_1 \oplus E_1$. The state transforming according to A_1 is clearly

$$|A_1\rangle = \frac{1}{\sqrt{3}}(|1\rangle + |2\rangle + |3\rangle).$$

The remaining two states transform according to E_1, and have the same energy. We cannot determine the relative energy levels using group theory, only the states themselves.

Example 5.7. When electron-electron interactions are ignored, electrons in atoms have the symmetry of $SO(3)$, the group of three-dimensional rotations. These representations are labeled by an integer j, and have dimension $2j + 1$. There is one conjugacy class for every distinct angle of rotation, and the characters of the jth representation are

$$\chi_j(\theta) = 1 + 2 \sum_{m=1}^{j} \cos(m\theta).$$

Assume a metal atom acquires six ligands in an octahedral orientation, reducing the full $SO(3)$ symmetry to O, the symmetry group of the cube. Use the following character table to determine how the five-fold degenerate $j = 2$ energy levels of the hydrogen atom split in the presence of

the ligands. The conjugacy classes are labeled by the angle of rotation. (Note that this type of level splitting is responsible for the vibrant colors in transition metal complexes, because of the wavelengths emitted with electrons transition between the split levels).

T	$0\,[1]$	$2\pi/3\,[8]$	$\pi\,[3]$	$\pi/2\,[6]$	$\pi\,[6]$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1

Solution: The relevant characters for the $j = 2$ representation of $SO(3)$ are

$$\begin{aligned}\chi_2(0) &= 1 + 2(\cos(0) + \cos(0)) = 5,\\ \chi_2(\pi/2) &= 1 + 2(\cos(\pi/2) + \cos(\pi)) = -1,\\ \chi_2(2\pi/3) &= 1 + 2(\cos(2\pi/3) + \cos(4\pi/3)) = -1,\\ \chi_2(\pi) &= 1 + 2(\cos(\pi) + \cos(2\pi)) = 1.\end{aligned}$$

Therefore, the character with respect to the conjugacy classes of T is $(5, -1, 1, -1, 1)$. Taking inner products with the characters of T, we find that the $j = 2$ representation of $SO(3)$ decomposes as $E \oplus T_2$. Therefore, the fivefold degenerate level splits into a twofold degenerate level transforming as E and a threefold degenerate level transforming as T_2. The magnitude of the energy difference depends on the metal and the ligand, but the number of states in each level is fixed by this simple group theoretic calculation.

6 Path Integral Formulation

A classic demonstration of wave-particle duality is the double-slit experiment. When electrons are fired through a screen containing two slits, they form an interference pattern on a detector wall behind the screen. This is attributed to the fact that the electrons are not at a fixed position, but rather have a wavefunction describing a distribution in space. The wavefunction can have nonzero amplitude for traveling between each slit, and so the two paths interfere on the detector screen, much the same way that classical waves interfere with themselves after diffracting through an obstacle.

The path integral formulation, originally developed by Richard Feynman, dramatically generalizes this idea so that all quantum dynamics can be thought of in terms of interfering paths. It is notoriously difficult to use the path integral to do actual calculations, but the path integral can provide qualitative understanding of quantum mechanics. In particular, we will use it to derive the action principle in classical mechanics, bringing our tour of quantum theory full circle. After this, we will explain the Aharanov-Bohm effect, and show that full circles are not always as they seem.

6.1 Action Principle

We will essentially follow Feynman's reasoning in constructing the path integral. In the double slit experiment, we sum over two classical paths (one for each slit). This divides the dynamics of the electron into two stages, before the slits and after the slits. We can express this division formally in the following way. We are attempting to compute the intensity pattern on the detector screen at position $\boldsymbol{x}_2$ after a time t, assuming the particle started at position $\boldsymbol{x}_1$ at time 0. We know that quantum states evolve by the unitary evolution $|\psi\rangle \mapsto e^{-i\hat{\mathcal{H}}t/\hbar}|\psi\rangle$, so the final state is $e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_1, 0\rangle$. The amplitude for this state to be at $|\boldsymbol{x}_2, t\rangle$ is

$$\langle \boldsymbol{x}_f, t|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_i, 0\rangle\,.$$

We call this object the *propagator*.

When we insert the double slit apparatus, we split the unitary evolution into two parts, and sum over the possible slits. The sum takes the form

$$\langle \boldsymbol{x}_f, t|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\text{slit 1}\rangle\,\langle\text{slit 1}|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\boldsymbol{x}_i, 0\rangle + \langle \boldsymbol{x}_f, t|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\text{slit 2}\rangle\,\langle\text{slit 2}|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\boldsymbol{x}_i, 0\rangle\,.$$

Of course, inserting the slits changes the dynamics, so we should not expect the two amplitudes we just wrote to be equal. However, nothing is stopping us from performing the same kind of manipulation even when no slits have been inserted. We could perform half of the time evolution, add up all the possible positions of the particle, and then perform the remainder. If we do this, then we should have an equality:

$$\langle \boldsymbol{x}_f, t|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_i, 0\rangle = \int d\boldsymbol{x}\;\langle \boldsymbol{x}_f, t|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\boldsymbol{x}, t/2\rangle\,\langle \boldsymbol{x}, t/2|e^{-i\hat{\mathcal{H}}(t/2)/\hbar}|\boldsymbol{x}_i, 0\rangle\,.$$

This is nothing new, algebraically: we are just inserting the complete set $|\boldsymbol{x}\rangle$. The new idea is to think of this operation as summing over classical states in the middle of the evolution.

So far, this manipulation hasn't simplified our problem. In fact, it has made it worse: instead of one propagator, we have two, and an integral over their product. Quantum mechanics is acting like the mythical Hydra, spawning two heads for every head we cut off. Thankfully, we can slay the Hydra. First, instead of splitting the evolution at a single time, we will split it at $N-1$ times, spaced by t/N. To simplify the notation, we will set $\boldsymbol{x}_0 = \boldsymbol{x}_i$ and $\boldsymbol{x}_N = \boldsymbol{x}_f$, and also suppress time labels in the states. This gives

$$\langle \boldsymbol{x}_N|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_0\rangle = \int d\boldsymbol{x}_1\cdots d\boldsymbol{x}_{N_1}\,\langle \boldsymbol{x}_N|e^{-i\hat{\mathcal{H}}t/N\hbar}|\boldsymbol{x}_{N-1}\rangle\,\langle \boldsymbol{x}_{N-1}|\cdots|\boldsymbol{x}_1\rangle\,\langle \boldsymbol{x}_1|e^{-i\hat{\mathcal{H}}t/N\hbar}|\boldsymbol{x}_0\rangle\,.$$

In order to make further progress, we need to evaluate objects of the form

$$\langle \boldsymbol{x}_{i+1}|e^{-i\hat{\mathcal{H}}t/N\hbar}|\boldsymbol{x}_i\rangle\,.$$

We will now make a crucial observation. It is not generally the case that $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}$; if $\hat{A}$ and $\hat{B}$ do not commute, then there will be additional terms related to their commutator. However, if

we let N grow large, then it is appropriate to use only the first term in the series expansion of the exponential, and so

$$e^{-i\hat{\mathcal{H}}t/N\hbar} \approx 1 - i\frac{\hat{\mathcal{H}}t}{N\hbar} \approx \left(1 - i\frac{\hat{p}^2 t}{2mN\hbar}\right)\left(1 - i\frac{V(\hat{x})t}{N\hbar}\right) \approx e^{-i\hat{p}^2 t/2mN\hbar} e^{-iV(\hat{x})t/N\hbar}.$$

These approximations become exact in the limit $N \to \infty$. Half of our job is done; we have

$$\langle \boldsymbol{x}_{i+1}|e^{-i\hat{\mathcal{H}}t/N\hbar}|\boldsymbol{x}_i\rangle = \langle \boldsymbol{x}_{i+1}|e^{-i\hat{p}^2 t/2mN\hbar} e^{-iV(\boldsymbol{x}_i)t/N\hbar}|\boldsymbol{x}_i\rangle\,.$$

Note that on the right hand side, the second factor is a number, not an operator. It is easy to evaluate an exponential of a function of the position operator when we are in the position basis. To evaluate the kinetic energy term, we convert to the momentum basis, obtaining finally

$$\begin{aligned}\langle \boldsymbol{x}_{i+1}|e^{-i\hat{\mathcal{H}}t/N\hbar}|\boldsymbol{x}_i\rangle &= \int d\boldsymbol{p}_i\ \langle \boldsymbol{x}_{i+1}|e^{-ip_i^2 t/2mN\hbar} e^{-iV(\boldsymbol{x}_i)t/N\hbar}|\boldsymbol{p}_i\rangle\,\langle \boldsymbol{p}_i|\boldsymbol{x}_i\rangle \\ &= \int d\boldsymbol{p}_i\, e^{-i\mathcal{H}(\boldsymbol{x}_i,\boldsymbol{p}_i)t/N\hbar}\,\langle \boldsymbol{x}_{i+1}|\boldsymbol{p}_i\rangle\,\langle \boldsymbol{p}_i|\boldsymbol{x}_i\rangle\end{aligned}$$

Applying the same method to every matrix element appearing in our integral, we find

$$\begin{aligned}\langle \boldsymbol{x}_N|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_0\rangle = \int d\boldsymbol{x}_1\cdots d\boldsymbol{x}_{N_1}\, d\boldsymbol{p}_0\cdots d\boldsymbol{p}_{N-1}\, e^{-i\mathcal{H}(\boldsymbol{x}_0,\boldsymbol{p}_0)t/N\hbar}\cdots e^{-i\mathcal{H}(\boldsymbol{x}_{N-1},\boldsymbol{p}_{N-1})t/N\hbar} \\ \langle \boldsymbol{x}_N|\boldsymbol{p}_{N-1}\rangle\,\langle \boldsymbol{p}_{N-1}|\boldsymbol{x}_{N-1}\rangle\cdots\langle \boldsymbol{x}_1|\boldsymbol{p}_0\rangle\,\langle \boldsymbol{p}_0|\boldsymbol{x}_0\rangle\,.\end{aligned}$$

We are now in a good position; we know the values of all the inner products appearing. Recall that

$$\langle \boldsymbol{x}|\boldsymbol{p}\rangle = e^{i\boldsymbol{x}\cdot\boldsymbol{p}/\hbar}.$$

It follows that

$$\langle \boldsymbol{x}_{i+1}|\boldsymbol{p}_i\rangle\,\langle \boldsymbol{p}_i|\boldsymbol{x}_i\rangle = e^{\frac{i}{\hbar}\boldsymbol{p}_i\cdot(\boldsymbol{x}_{i+1}-\boldsymbol{x}_i)}.$$

Using this relation N times in the above integral, we arrive at

$$\begin{aligned}\langle \boldsymbol{x}_N|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_0\rangle = \int d\boldsymbol{x}_1\cdots d\boldsymbol{x}_{N_1}\, d\boldsymbol{p}_0\cdots d\boldsymbol{p}_{N-1}\, e^{-i\mathcal{H}(\boldsymbol{x}_0,\boldsymbol{p}_0)t/N\hbar}\cdots e^{-i\mathcal{H}(\boldsymbol{x}_{N-1},\boldsymbol{p}_{N-1})t/N\hbar} \\ e^{\frac{i}{\hbar}\boldsymbol{p}_{N-1}\cdot(\boldsymbol{x}_N-\boldsymbol{x}_{N-1})}\cdots e^{\frac{i}{\hbar}\boldsymbol{p}_0\cdot(\boldsymbol{x}_1-\boldsymbol{x}_0)}.\end{aligned}$$

At this point, the Hydra is slain: everything appearing on the right hand side is a classical variable. This is the primary theoretical appeal of the path integral.

We can still do a great deal to simplify this expression. Since everything is classical, we can combine products of exponentials in the usual way, obtaining

$$\langle \boldsymbol{x}_N|e^{-i\hat{\mathcal{H}}t/\hbar}|\boldsymbol{x}_0\rangle = \int d\boldsymbol{x}_1\cdots d\boldsymbol{x}_{N_1}\, d\boldsymbol{p}_0\cdots d\boldsymbol{p}_{N-1}\, \exp\left[\frac{i}{\hbar}\sum_{i=0}^{N-1}\left(\boldsymbol{p}_i(\boldsymbol{x}_{i+1}-\boldsymbol{x}_i) - \mathcal{H}(\boldsymbol{x}_i,\boldsymbol{p}_i)\frac{t}{N}\right)\right].$$

The sum appearing in the exponential is, in fact, a Riemann sum. We can see this more clearly by factoring out $\Delta t = \frac{t}{N}$, to give

$$\sum_{i=0}^{N-1}\left(\boldsymbol{p}_i\frac{\boldsymbol{x}_{i+1}-\boldsymbol{x}_i}{\Delta t} - \mathcal{H}(\boldsymbol{x}_i,\boldsymbol{p}_i)\right)\Delta t.$$

In the limit $N \to \infty$, $\frac{\boldsymbol{x}_{i+1}-\boldsymbol{x}_i}{\Delta t} \to \dot{x}_{i+1}$, and the sum becomes the integral

$$\int_0^t (\boldsymbol{p} \cdot \dot{\boldsymbol{x}} - \mathcal{H})\, dt.$$

Now, recall from Section 1 the definition of the Hamiltonian:

$$\mathcal{H} = \boldsymbol{p} \cdot \dot{\boldsymbol{x}} - \mathcal{L}.$$

Substituting this, we find that the integral is none other than

$$\int_0^t \mathcal{L}\, dt = S,$$

the action.

Putting this back into our expression for the propagator, we find

$$\langle \boldsymbol{x}_f | e^{-i\hat{\mathcal{H}}t/\hbar} | \boldsymbol{x}_i \rangle = \int \mathcal{D}x(t)\, e^{\frac{i}{\hbar}S[x(t)]},$$

where the differential $\mathcal{D}x(t)$ represents the $N \to \infty$ limit of the variables $d\boldsymbol{x}_1 \cdots d\boldsymbol{x}_{N_1}\, d\boldsymbol{p}_0 \cdots d\boldsymbol{p}_{N-1}$, i.e., the position and momentum at every point along a classical path. We have found that the amplitude for a quantum particle to travel from $\boldsymbol{x}_i$ to $\boldsymbol{x}_f$ is given by an integral over all classical paths, weighted by a phase factor related to the classical action.

This equation begs the question of why we do not see the effects present in the double-slit experiment in everyday life. When you throw a baseball, it does not explore all possible paths and diffract with itself in a wavelike manner; it acts like a classical particle. Put another way, it follows a path of stationary action. We can understand this using the path integral. As $\hbar \to 0$ (i.e., the classical limit), any paths which do not have stationary action are strongly suppressed in the path integral. This happens because, in the space of nearby paths, the action changes linearly, and so the phase $\frac{i}{\hbar}S[x(t)]$ changes rapidly. Integrating a rapidly oscillating phase gives zero. However, if the path $x_{\mathrm{cl}}(t)$ has stationary action, then the integral over nearby paths gives a large amplitude proportional to $e^{\frac{i}{\hbar}S[x_{\mathrm{cl}}(t)]}$. Thus, in the classical limit, particles follow only paths of stationary action.

6.2 Aharanov-Bohm Effect

The path integral is a useful way of understanding some confusing effects in quantum theory. One of these is the Aharanov-Bohm effect. This section will only give a sketch of the physics involved here, and should be taken as an invitation to study gauge theory in greater detail.

Consider a classical particle with charge q in an electromagnetic field, given by

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}, \qquad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$$

where ϕ and $\boldsymbol{A}$ are the electric and magnetic potentials respectively. Crucially, these potentials are not physical, classically. They have a redundancy known as *gauge symmetry*: by changing

$$\phi \mapsto \phi - \frac{1}{c}\frac{\partial \chi}{\partial t}, \qquad \boldsymbol{A} \mapsto \boldsymbol{A} + \boldsymbol{\nabla}\chi,$$

we do not change the physical $\boldsymbol{E}$ and $\boldsymbol{B}$ fields.

It is not obvious how to form a Lagrangian, since the Lorentz force is velocity-dependent:

$$\boldsymbol{F} = q\left(\boldsymbol{E} + \frac{\dot{\boldsymbol{x}}}{c} \times \boldsymbol{B}\right) = q\left(-\boldsymbol{\nabla}\phi - \frac{1}{c}\frac{d\boldsymbol{A}}{dt} + \frac{1}{c}\boldsymbol{\nabla}(\boldsymbol{v}\cdot\boldsymbol{A})\right).$$

The second equality is nontrivial; you are encouraged to apply cross product identities and work it out for yourself. It turns out that the correct Lagrangian is

$$\mathcal{L}(\boldsymbol{x}, \dot{\boldsymbol{x}}) = \frac{1}{2}m\dot{x}^2 - q\phi(\boldsymbol{x}) + \frac{q}{c}\dot{\boldsymbol{x}}\cdot\boldsymbol{A}.$$

To see this, we form the Euler-Lagrange equations:

$$\frac{d}{dt}\left(m\dot{\boldsymbol{x}} + \frac{q}{c}\boldsymbol{A}\right) + q\left(\boldsymbol{\nabla}\phi - \frac{1}{c}\boldsymbol{\nabla}(\boldsymbol{v}\cdot\boldsymbol{A})\right) = 0.$$

Rearranging this gives the Lorentz force law as written above.

Example 6.1. Determine the Hamiltonian for a particle in an electromagnetic field, and use the Schrödinger equation to show that a wavefunction acquires a phase $e^{\frac{iq}{\hbar c}\int_\gamma \boldsymbol{A}\cdot d\boldsymbol{x}}$ as it moves along a path γ.

Solution: The canonical momentum is not the usual $m\dot{\boldsymbol{x}}$, but rather

$$\boldsymbol{p} = m\dot{\boldsymbol{x}} + \frac{q}{c}\boldsymbol{A}.$$

The Hamiltonian is then

$$\mathcal{H} = \boldsymbol{p}\cdot\dot{\boldsymbol{x}} - \mathcal{L} = \frac{1}{2}m\dot{x}^2 + q\phi(\boldsymbol{x}) = \frac{\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}\right)^2}{2m} + q\phi(\boldsymbol{x}).$$

The Schrödinger equation for the wavefunction reads

$$\left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - \frac{q}{c}\boldsymbol{A}\right)^2 + q\phi(\boldsymbol{x})\right]\psi(\boldsymbol{x}) = E\psi(\boldsymbol{x}).$$

Consider the adjusted wavefunction $\tilde{\psi}$ defined by

$$\psi(\boldsymbol{x}) = e^{\frac{iq}{\hbar c}\int_\gamma \boldsymbol{A}\cdot d\boldsymbol{x}}\tilde{\psi}(\boldsymbol{x}).$$

Substituting this expression into the Schrödinger equation, we find

$$\left[-\frac{\hbar^2\boldsymbol{\nabla}^2}{2m} + q\phi(\boldsymbol{x})\right]\tilde{\psi}(\boldsymbol{x}) = E\tilde{\psi}(\boldsymbol{x}).$$

Therefore, $\tilde{\psi}(\boldsymbol{x})$ satisfies the "normal" Schrödinger equation, and this establishes that $\psi(\boldsymbol{x})$ acquires the given phase factor relative to its counterpart that does not see a magnetic potential.

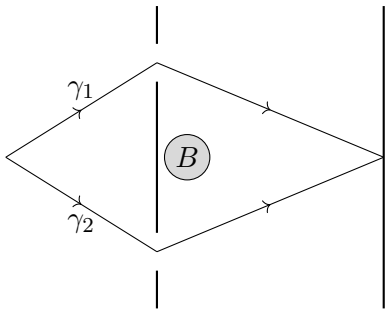


Figure 5: In the Aharanov-Bohm effect, particles acquire a phase factor while moving around a solenoid.

The same result can be obtained much more easily using the path integral. The action can be written as

$$S[x(t)] = S_{\boldsymbol{A}=0}[x(t)] + \int_0^t \frac{q}{c}\dot{\boldsymbol{x}} \cdot \boldsymbol{A}\, dt = S_{\boldsymbol{A}=0}[x(t)] + \frac{q}{c}\int \boldsymbol{A} \cdot d\boldsymbol{x},$$

and the second factor accounts for the extra phase in the wavefunction.

The vector potential gives rise to the magnetic field, but it can be nonzero even in regions of vanishing magnetic field. For example, in a solenoid of radius r_s oriented along the z axis at the origin, the magnetic field is $\boldsymbol{B} = B_z\hat{\boldsymbol{z}}$ inside the coil, and vanishes outside. But the vector potential is given by

$$\boldsymbol{A} = \begin{cases} \frac{Br}{2}\hat{\boldsymbol{\theta}} & \text{if } r < r_s \\ \frac{Br_s^2}{2r}\hat{\boldsymbol{\theta}} & \text{otherwise} \end{cases}.$$

It does not vanish anywhere.

We can now describe the Aharanov-Bohm experiment. It is very similar to the double-slit experiment, except a solenoid is inserted behind the slits, as shown in Figure 5. The interference pattern in the classic double-slit experiment is set by the relative phase of electrons traveling through the two slits. Since the vector potential is nonzero even outside the solenoid, the interference pattern may be changed by the presence of the solenoid, even though classically the particles would never experience the magnetic field.

If we label the top path by γ_1 and the bottom path by γ_2, as in Figure 5, then the added relative phase factor between the two paths is

$$e^{\frac{iq}{\hbar c}\left(\int_{\gamma_1} \boldsymbol{A}\cdot d\boldsymbol{x} - \int_{\gamma_2} \boldsymbol{A}\cdot d\boldsymbol{x}\right)} = e^{\frac{iq}{\hbar c}\oint \boldsymbol{A}\cdot d\boldsymbol{x}}.$$

While $\boldsymbol{A}$ is a gauge-dependent quantity, its loop integral is gauge-invariant. We can see this by performing a gauge transformation:

$$\oint \boldsymbol{A} \cdot d\boldsymbol{x} \mapsto \oint (\boldsymbol{A} + \boldsymbol{\nabla}\chi) \cdot d\boldsymbol{x} = \oint \boldsymbol{A} \cdot d\boldsymbol{x},$$

since the loop integral of a gradient vanishes. In fact, the loop integral of $\boldsymbol{A}$ has a direct physical meaning, via Stokes' theorem:

$$\oint \boldsymbol{A} \cdot d\boldsymbol{x} = \iint (\boldsymbol{\nabla} \times \boldsymbol{A}) \cdot d\boldsymbol{S} = \iint \boldsymbol{B} \cdot d\boldsymbol{S},$$

the magnetic flux. Thus, the difference in phase of the two electrons is shifted by $\frac{q\Phi_B}{\hbar c}$ when the solenoid is inserted. This leads to a visible shift in the interference pattern on the detector.

Example 6.2. Show that the time-dependent Schrödinger equation of a particle in an electromagnetic field is gauge invariant if the gauge transformations are amended to include a phase shift in the wavefunction.

Solution: Applying a gauge transformation to the time-dependent Schrödinger equation, we have

$$\left[-\frac{\hbar^2}{2m}\left(-i\hbar\boldsymbol{\nabla}-\frac{q}{c}(\boldsymbol{A}+\boldsymbol{\nabla}\chi)\right)^2+q\left(\phi-\frac{1}{c}\frac{\partial\chi}{\partial t}\right)\right]e^{i\lambda}\psi(\boldsymbol{x})=i\hbar\frac{d}{dt}\left(e^{i\lambda}\psi(\boldsymbol{x})\right),$$

where λ is some phase factor depending on the gauge function χ. If the Schrödinger equation is to be gauge invariant, we must satisfy

$$\left(-i\hbar\boldsymbol{\nabla}-\frac{q}{c}\boldsymbol{\nabla}\chi\right)e^{i\lambda}=0,$$
$$i\hbar\frac{d}{dt}e^{i\lambda}=-\frac{q}{c}\frac{\partial\chi}{\partial t}e^{i\lambda}.$$

These equations are both satisfied by $\lambda=\frac{q}{\hbar c}\chi$. Therefore, the gauge transformation takes

$$\psi(\boldsymbol{x})\mapsto e^{\frac{iq}{\hbar c}\chi}\psi(\boldsymbol{x}),$$

in addition to the usual transformations of ϕ and $\boldsymbol{A}$.