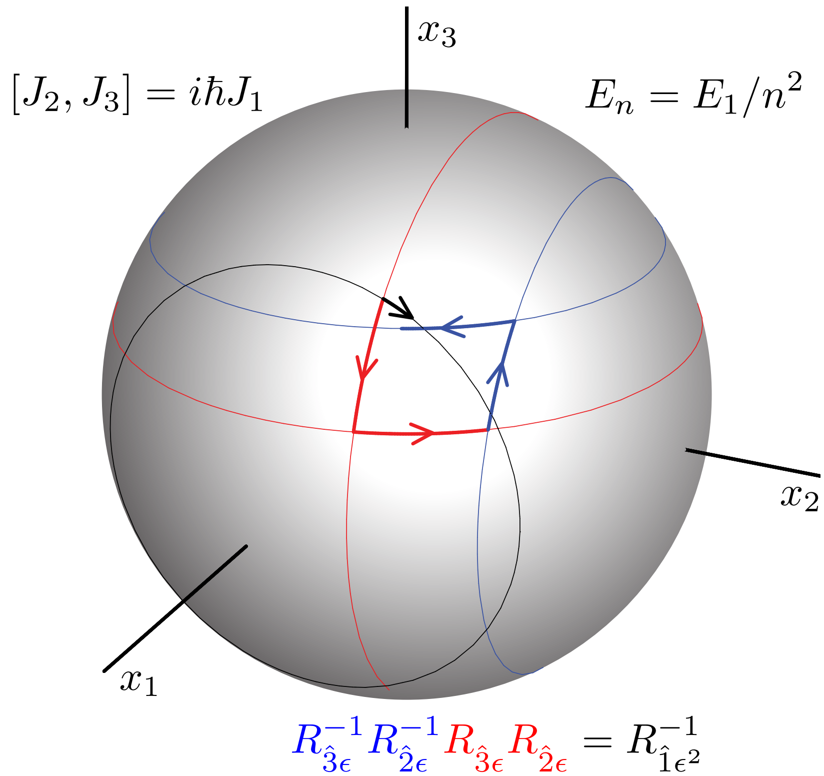

Introduction to Quantum Mechanics

From Geometry to Spectra

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Chapter 1

Quantum Phenomenology

Of the two great physics revolutions of the early 1900s, relativity "completes" classical physics, but quantum physics subsumes it.

Richard Feynman wrote, "Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen"[1].

One can't learn about atoms by playing with billiard balls, but one can learn about billiard balls by studying atoms. Classical physics follows from quantum physics, not the other way around.

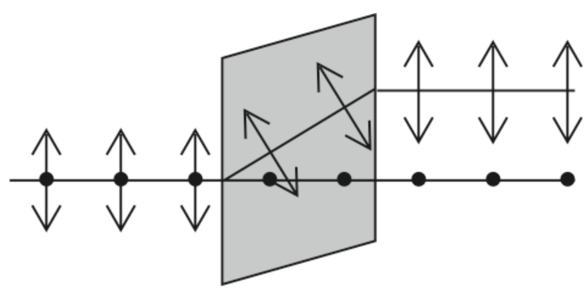


Figure 1.1: A calcite crystal sorts classical light into vertical (up-down arrows) and horizontal (in-out dots) polarizations. Thus, a black disk seen through calcite would appear as two gray disks.

1.1 Preamble: Sorting Photons

Optically anisotropic materials can sort light according to its polarization (the oscillation direction of its electric field). For example, because of its crystal structure, calcite is *birefringent* with different indices of refraction for electric fields perpendicular and parallel to its optic axis, as illustrated in Fig. 1.1. Schematically represent the action of the calcite by a box with one input and two outputs, as in Fig. 1.2. Convert a vertical and horizontal $\oplus$ sorter into a $\pm 45°$ diagonal $\otimes$ sorter by rotating the calcite. For bright classical light, if diagonally polarized light is input to a $\oplus$ sorter, then half of the input light intensity will appear in each output channel. Similarly, if vertically polarized light is input to a $\otimes$ sorter, then half of the input light intensity will appear in each output channel.

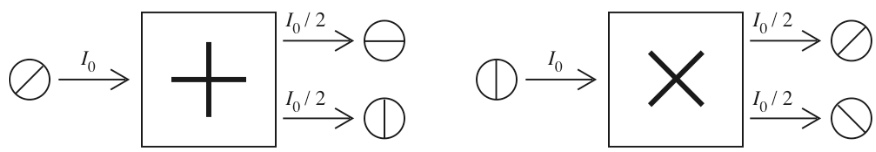


Figure 1.2: Diagonally polarized light input to a $\oplus$ sorter (left) and vertically polarized light input to a $\otimes$ sorter (right).

Repeat this experiment with very faint light. What happens? Near the beginning of the twentieth century, the Einstein photoelectric effect and the Compton scattering experiment demonstrated the "granularity" of faint light. In fact, they suggested that light consists of particles whose energy is proportional to the light's classical temporal frequency

$$E = \hbar\omega, \tag{1.1}$$

whose momentum is proportional to the light's classical spatial frequency

$$\vec{p} = \hbar\vec{k}, \tag{1.2}$$

and whose spin angular momentum corresponds to the light's classical (circular) polarization

$$\vec{\mathscr{S}} = \pm\hbar\hat{k}, \tag{1.3}$$

where the common proportionality $\hbar = h/2\pi$ is Planck's (reduced) constant. These particles are now called *photons*. Classical wave-like light emerges from a large ensemble of particle-like photons. Electrons and other subatomic particles (and even atoms and molecules . . .) exhibit similar *wave-particle duality*. Such "wavicles" or "matter-waves" have been called "the dreams stuff is made of" [2].

Use neutral density filters (NDFs) to reduce the intensity of the light so that there is only one photon in the sorter at any one time. To count the photons in each of the output channels, use photomultiplier tubes (PMTs), which exploit the photoelectric effect to convert a single photon into a macroscopic cascade of electrons. (Alternately, use a frog's eye, which is apparently sensitive to single photons!) For each experimental trial, each PMT will report "1" if it detects a photon and "0" if it does not.

Input a diagonally polarized photon to a $\oplus$ sorter. What happens? The input photon must emerge in one of the two output channels, if only because it must go somewhere, but why would it emerge in one channel and not the other? In fact, as illustrated in Fig. 1.3, the experiment is *not* repeatable, which is itself a disaster for classical physics; rather, the photon emerges half the time in each channel, *randomly*. It is impossible to predict in which output channel any given input photon will emerge, but it is possible to predict the *probability* that it will emerge in either channel, and the equal probabilities of 1/2 correspond well with the classical, bright-light result. The *indeterminism* of the individual trials of this experiment is in striking disagreement with classical physics and is a hallmark of quantum mechanics.

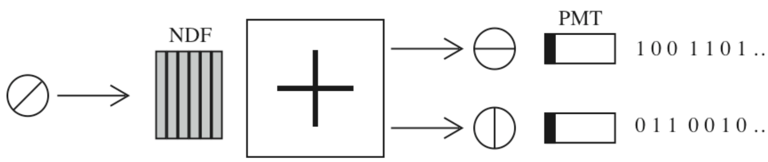


Figure 1.3: Diagonally polarized photons input to a ⊕ sorter emerge randomly but equally in each output channel. Neutral density filters (left) reduce the input intensity of the light to single photons at a time, while photomultipliers (right) count the output photons.

Next recombine the two output channels with a reversed ⊕ sorter, as in Fig. 1.4. Now the experiment is repeatable and determined! If the ⊕ sorter randomizes the diagonal polarization, how does the recombination preserve it? Surely, the diagonally polarized photon entering the first ⊕ sorter can not "know" it will be recombined by the second, reversed ⊕ sorter?

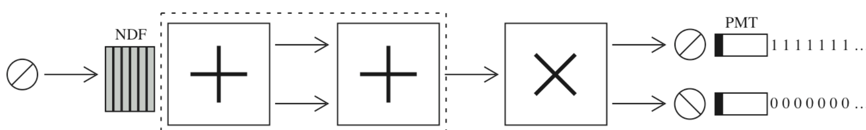


Figure 1.4: One ⊕ sorter randomizes the diagonal polarization but adding a second, reversed ⊕ sorter *preserves* the diagonal polarization.

Classically, the diagonal light can be thought of as a *superposition* of horizontal and vertical light and constructive *interference* between the two channels can preserve its polarization. Interference and superposition are keys to understanding quantum phenomena.

1.2 Interference & Superposition

The quantum analogues of the classic wave concepts of interference and superposition reveal deep and surprising features of quantum reality.

1.2.1 Beam Splitter Probabilities

A beam splitter is an optical device that transmits half the light incident on it and reflects the other half. It could be a mirror with an unusually thin metal layer or a dielectric slab whose thickness and index of refraction together produce the desired constructive and destructive interference. Imagine it to be two prisms separated by a small gap, as in Fig. 1.5. Varying the thickness of the spacer, a thin film that separates the two prisms, can produce any ratio of transmitted to reflected light, via an exponentially decaying *evanescent wave* propagating through the spacer, a phenomenon called *frustrated total internal reflection*.

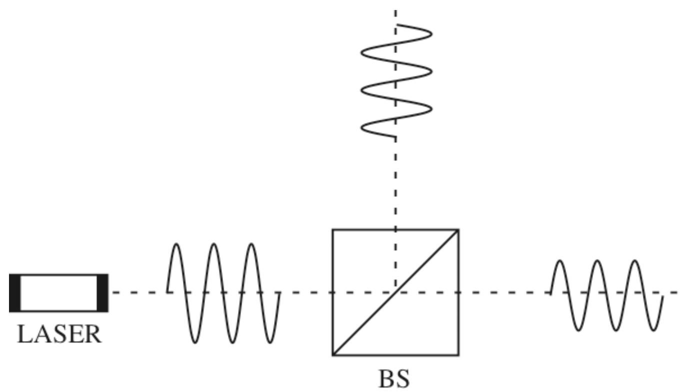


Figure 1.5: Beam splitter reduces the reflected and transmitted bright light intensity by 1/2 and amplitude by $1/\sqrt{2}$.

For simplicity, imagine that the light source is monochromatic. This could be a laser, which consists of an electrically excited medium bounded by two mirrors, one of which is partially reflecting. De-excitation results in monochromatic, coherent, and directional light escaping the partially reflecting mirror.

At sufficiently high intensity, light behaves like an electromagnetic wave. The frequency of visible light is so high ($\nu = \omega/2\pi \sim 100\text{THz}$) that human eyes and cameras cannot follow its oscillations. Instead, eyes and cameras are sensitive to the time averaged square of its electric field, which is called *intensity* (or *irradiance*). Intensity is the energy per unit area per unit time transported by the wave. If the electric field varies sinusoidally, $\mathcal{E} = \mathcal{E}_0 \cos[kx - \omega t]$, then its intensity is proportional to the electric field amplitude squared, $I \propto \langle \mathcal{E}^2 \rangle \propto \mathcal{E}_0^2$. In appropriate units, take $I = \mathcal{E}_0^2$. Thus, in reducing the intensity of the transmitted and reflected waves by 1/2, the beam splitter of Fig. 1.5 reduces the electric field amplitude by $1/\sqrt{2}$.

At sufficiently low intensity, the graininess of light becomes apparent, and light behaves like a stream of particles, called photons. The energy of single visible-light photons is so small ($E = h\nu \sim 1\text{eV}$) that human eyes are not (quite)

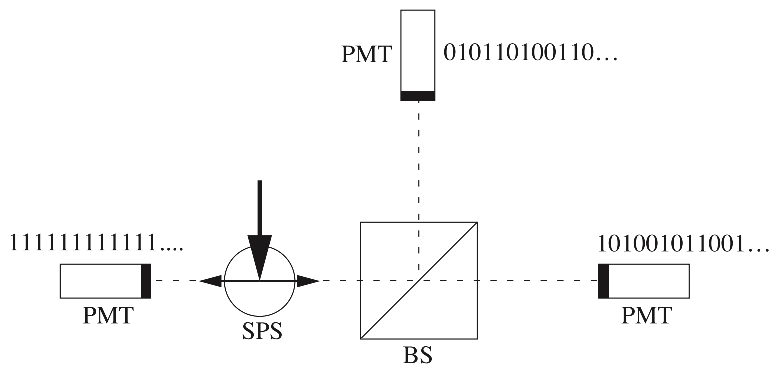


Figure 1.6: Beam Splitter reflects and transmits photons with probability 1/2. For each trial, each PhotoMultiplier Tube reports “1” if it detected a photon and “0” otherwise. Single Photon Source produces a pair of opposing photons so that one enters the Beam Splitter and the other announces the trial.

able to detect them. Instead, detect them with either analog photomultiplier tubes (PMTs) or semiconductor avalanche photodiodes (APDs), which exploit the photoelectric effect to initiate an electron cascade that amplifies a single photoelectron to a macroscopic current pulse with near 100% efficiency.

Radically dim the light source using neutral density filters (NDFs) or crossed polarizers, so that there is only one photon in the beam splitter at any one time, on average. To avoid photon bunching, use a single photon source. For example, wait for positronium to decay into opposing photons and detect one to herald the other. More practically, pump a nonlinear birefringent crystal, like β-BaB_2O_4 (BBO), with a UV laser to produce two opposing IR photons and again detect one to announce the other.

What happens in repeated trials at the beam splitter? If the first photon is reflected, shouldn't they all be reflected? If the first is transmitted, shouldn't they all be transmitted? How then can the bright light classical results emerge from the faint light quantum results by gradually increasing the light intensity?

Put nature to the test – and find that the experiment is *not repeatable*. Instead, individual photons are transmitted or reflected with probability 1/2, as in Fig. 1.6, where the binary data strings at each PMT indicate whether a photon has been detected (1) or not (0) during each trial. More generally, find that the probability of detecting a photon is proportional to the square of the amplitude of the electric field of the corresponding classical wave. In this way, faint light quantum experiments *correspond* to bright light classical experiments.

1.2.2 Two Interpretations

The conventional or *Copenhagen* interpretation (CI) is that quantum probabilities are *ontological* rather than *epistemological*. They reflect how things really are, not merely what can be known about them. They are inherent in nature, not merely limitations in the measuring apparatus.

Einstein famously objected, “God does not play dice with the universe”.

In the post-Einstein *Many Worlds* interpretation (MWI), the ontological probabilities are eliminated. Instead, each photon is both transmitted *and* reflected, and the world splits into two histories, one for each possibility! Epistemological randomness is apparent only to observers, like physicists, confined to single histories. From a God’s eye perspective, the MWI is deterministic and, for the beam splitter, symmetric (both of two equally likely possibilities are realized), but at the ontological expense of invoking an uncountable infinity of equally real worlds to explain the single observable world.

There are other interpretations, but none preserve classical reality.

1.2.3 Mach-Zehnder Interferometer

Probabilities alone don’t exhaust the novelty of quantum reality.

Recombine the light from a beam splitter using two mirrors and a second beam splitter, as in Fig. 1.7. Such a device is called a *Mach-Zehnder* interferometer. If “T” and “R” represent “transmitted” and “reflected”, then the four paths through the interferometer can be denoted RRR, TRT, RRT, TRR, where the first two paths exit up and the second two paths exit right. All paths have the same length, but each transmission and reflection is accompanied by a phase shift that depends on the details of the optics. However, light waves *interfere* constructively when exiting right (and, by energy conservation, destructively when exiting up), because the corresponding paths involve the same number of transmissions and the same number of reflections. (In practice, a dielectric slab in one path of the interferometer can be rotated slightly to adjust the phase shifts. Also, if one of the mirrors or beam splitters is slightly canted, then the interference produces a fringe pattern of parallel stripes.)

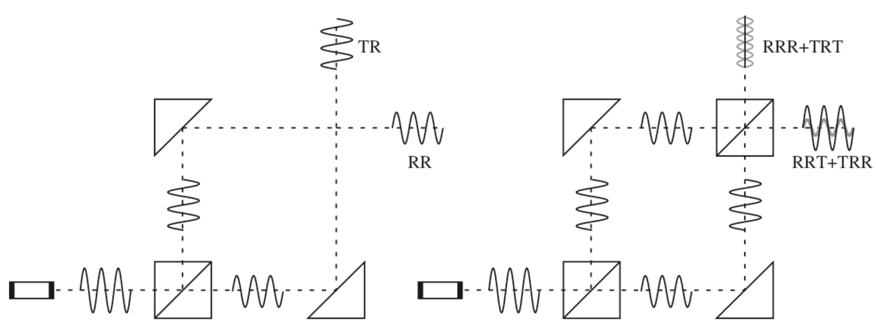


Figure 1.7: Mirrors (left) and a second beam splitter (right) recombine bright light split by the first beam splitter.

Radically dim the light source so that only one photon is in the interferometer at any one time, as in Fig. 1.8. What happens? Without the recombining beam splitter, the data strings at the PMTs are perfectly anticorrelated but random. With the recombining beam splitter, the data strings are still perfectly anticorrelated but are now homogeneous, and all photons exit right, in agreement with the high intensity experiment. Apparently, there is interference even with only one photon in the apparatus at a time!

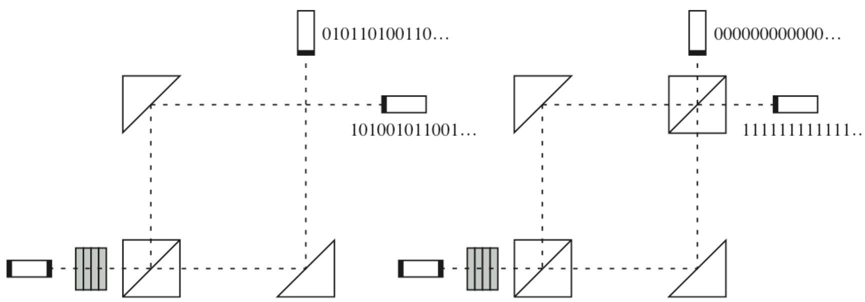


Figure 1.8: Mirrors (left) and a second beam splitter (right) recombine photon paths split by the first beam splitter.

Note how the addition of the recombining beam splitter radically alters the output of the device. If individual photons were somehow "splitting" (or not) at the first beam splitter, how could they know whether (or not) the recombining beams splitter was in place? In fact, since the speed of the photons is $c \sim 10^9$ km/hr ~ 0.3 m/ns, nanosecond electronics in a table-top experiment can decide to remove or introduce the recombining beam splitter *after* the photon has interacted with the first beam splitter! The results of such *delayed choice* experiments are exactly the same: in those trials with the recombiner, all photons exit right; in those trials without the recombiner, half the photons exit right and half exit up.

Try to check the paths taken by the photons. Since each photon carries momentum $p = h/\lambda$, if one of the two mirrors floats or glides on a low-friction surface, then the mirror's recoil (or not) reveals the photon's path. However, in such *which-way* experiments, the constructive and destructive interference, which makes all photons exit right and none exit up, is destroyed, and instead half the photons exit right and half exit up. Indeed, which-way information is consistent with the particle nature of light but is inconsistent with the wave nature of light. Particles take definite paths and do not interfere, while waves take all paths and do interfere. Apparently, *incompatible* experimental arrangements elicit *complementary* aspects of the wave-particle duality of light: which-way information (no recombiner or floating mirrors) elicits the particle aspect of light, while no which-way information (recombiner and fixed mirrors) elicits the wave aspect of light.

1.2.4 Quantum Eraser

A *quantum eraser* is a measurement that destroys which-way information [3]. Because the eraser can *restore* an interference pattern, Neils Bohr's classic argument that the interference pattern is lost because it has been randomly disrupted by the measurement process is not applicable. Insert a 0° (horizontal) polarizer in one path of the Mach-Zehnder interferometer, a 90° (vertical) polarizer in the other path, a 45° (diagonal) polarizer at the input, and final (analyzing) polarizers at the outputs, as in Fig. 1.9. The path polarizers encode which-way information in a photon by altering its spin angular momentum, the quantum counterpart to the polarization of the corresponding classical wave, while not changing its linear momentum. (Floating one of the mirrors and observing it recoil obtains which-way information *at the expense of* changing the photon's linear momentum, but floating one of the mirrors and observing it *not* recoil obtains which-way information *without* affecting the photon.)

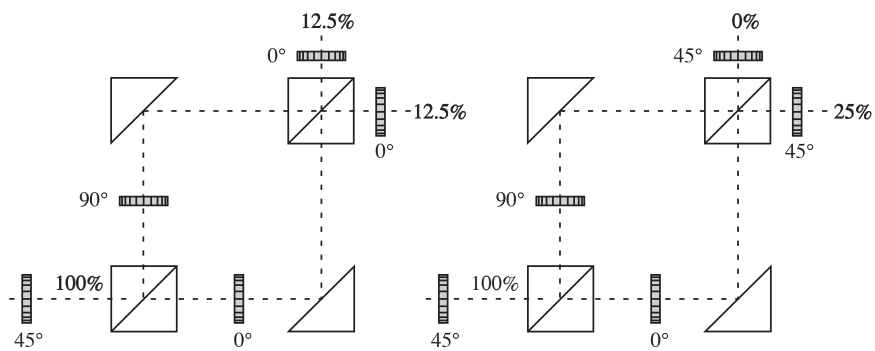


Figure 1.9: Path polarizers provide which-way information and interference is lost (left diagram), where photons exit equally up and right. Rotating the final, analyzing polarizers 45° destroys the which-way information and restores the interference (right diagram), where photons exit right but not up.

Rotate the analyzers to 0° and observe light propagating in only one path of the interferometer, so there is no interference, and half the photons exit right and half exit up. Rotate the analyzers to 90° and obtain similar results. Remove the analyzers and still observe no interference. Apparently, it is not necessary to actually detect a particular path, as merely encoding which-way information is sufficient to destroy the interference. However, rotate the analyzers to 45°, so 0° (horizontal) and 90° (vertical) polarizations are no longer distinguishable, which-way information is erased, all photons exit right, and interference is restored – and this is so even if the quantum erasure is a delayed choice!

1.2.5 Interaction-Free Measurement

Floating one of the two mirrors in the Mach-Zehnder interferometer loses single-photon interference, even if the single photon reflects off the other, stationary mirror. How can the floating mirror affect the photon if the photon doesn't even come near it or exchange energy with it? Quantum physics allows us to test *counterfactuals*, things that might have happened but did not!

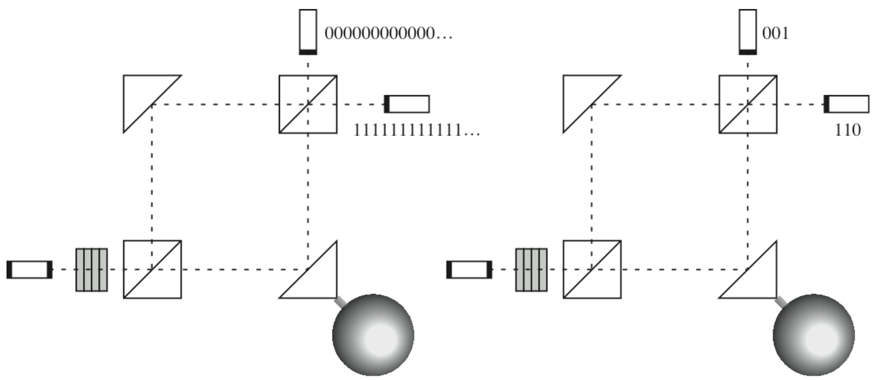


Figure 1.10: Interference (left) reveals a jammed detonator (and a fixed mirror), while no interference (right) reveals a working detonator (and a recoilable mirror).

The bomb testing problem of Avshalom Elitzur and Lev Vaidman [4] dramatically illustrates such *interaction-free* or *null* measurements. Consider bombs so sensitive that even the slightest movement of their detonators will explode them. Unfortunately, some fraction of the detonators are jammed and the attached bombs are consequently duds. Classically, there is no way to identify good bombs without exploding them, but quantum physics provides a way. Test a bomb by attaching its detonator to one of the mirrors of the Mach-Zehnder interferometer, as in Fig. 1.10.

If all photons exit right, the different alternatives are interfering, constructively right and destructively up. The mirror and its attached detonator must be fixed, so there is no which-way information. Hence, the bomb is a dud. However, if even one photon exits up, the different alternatives are not interfering. The mirror and the attached detonator can, in principle, recoil and thereby provide which-way information. Hence, the bomb is good, and if the photons have all reflected off the stationary mirror, the bomb is unexploded.

In practice, this scheme harvests only

$$\frac{1}{4}+\frac{1}{16}+\frac{1}{64}+\cdots=\frac{1}{3} \tag{1.4}$$

of the working bombs. However, a variation of this technique can arbitrarily reduce the fraction of wasted bombs.

1.2.6 Quantum Computing

Classically, distinguishing a real coin, with a head and a tail, from a trick coin, with two heads (or two tails) requires looking at each side separately and then comparing the results. However, David Deutsch's "two-bit" quantum algorithm can do this all at once!

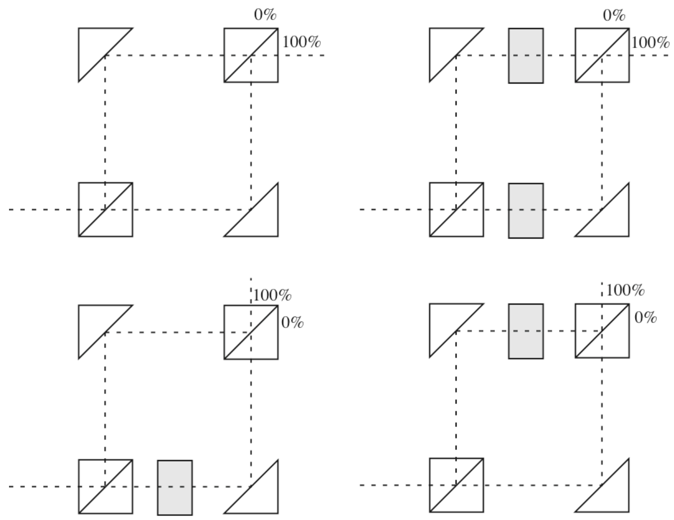


Figure 1.11: An "inverting" (π-phase shifting) dielectric is in one or both paths of the interferometer. If the photon exits right (top row), the paths are identical. If it exits up (bottom row), the paths are nonidentical.

As a slightly simplified quantum version of the problem, suppose that there may or may not be a piece of π-phase-shifting dielectric in one or both paths of a Mach-Zehnder interferometer, as in Figure 1.11. Classically, the presence of the dielectric in one path but not the other converts, at the exit, constructive interference to destructive interference, and vice versa. Quantumly, a single photon explores both paths in parallel. If it exits right instead of up, then both paths are the same, and one photon has obtained two bits of information.

Deutsch's 1985 two-bit scheme [5] was the first *quantum computing* algorithm. In 1994, Peter Shor discovered [6] a quantum computing algorithm to factor numbers in polynomial time, so that factoring an N-bit number requires time $O[N^k]$, for constant k. This is something no classical computer can do. Shor's algorithm would revolutionize cryptography, if robustly implemented. (In 2001, an early quantum computer ran Shor's algorithm and successfully factored $15 = 3 \times 5$, while in 2012, another quantum computer factored $21 = 3 \times 7$.) In 1996, Lov Grover discovered [7] a quantum computing algorithm to search a database of N elements in time $O[\sqrt{N}]$, again faster than any classical computer, which requires time $O[N]$.

The MWI provides an easy heuristic for understanding the source of the advantage of these quantum algorithms: they distribute the calculations among many parallel universes!

1.2.7 Mach-Zehnder Classical Model

Prior to creating a more explicit quantum model of the Mach-Zehnder interferometer, first create a more quantitative classical model. At high intensity, light is split into two wave trains at the first beam splitter, which are recombined at the second beam splitter and exit up and right. Let the electric field magnitude at the entrance be

$$\mathcal{E}[0,t] = \mathcal{E}_0 \cos[\omega t], \tag{1.5}$$

where t is the time elapsed, and $\omega = 2\pi/T$ is the temporal frequency of the wave train. Then, the electric field magnitude at the exit due to the wave train reflected by mirror n is

$$\mathcal{E}_n[z,t] = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\mathcal{E}_0 \cos[\omega t - kz + \delta_n], \tag{1.6}$$

where $z = 2\ell$ is the distance traveled, $k = 2\pi/\lambda$ is the spatial frequency, and δ_n is the extra phase shift due to reflections. Since $\omega/k = \lambda/T = c$, the spacetime phase $\varphi = \omega t - kz = k(ct - z)$ is zero at $z = ct$, and hence represents a wave traveling in the $\hat{z}$ direction at speed c. The factors of $1/\sqrt{2}$ are due to the beam splitters. The total electric field magnitude at the exit is the superposition

$$\mathcal{E} = \mathcal{E}_1 + \mathcal{E}_2 = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{2}}\mathcal{E}_0(\cos[\varphi + \delta_1] + \cos[\varphi + \delta_2]). \tag{1.7}$$

Eyes and cameras are sensitive to the time-averaged square of this electric field, which is the intensity

$$I = \langle \mathcal{E}^2 \rangle = \frac{1}{2}\frac{1}{2}\left\langle \mathcal{E}_0^2 \left(\cos^2[\varphi + \delta_1] + 2\cos[\varphi + \delta_1]\cos[\varphi + \delta_2] + \cos^2[\varphi + \delta_2]\right)\right\rangle . \tag{1.8}$$

Using the trigonometric identity $2\cos u \cos v = \cos[u+v] + \cos[u-v]$, this becomes

$$I = \frac{1}{2}\mathcal{E}_0^2 \frac{\left\langle \cos^2[\varphi + \delta_1]\right\rangle + \left\langle \cos[2\varphi + \delta_1 + \delta_2]\right\rangle + \left\langle \cos[\delta_1 - \delta_2]\right\rangle + \left\langle \cos^2[\varphi + \delta_2]\right\rangle}{2}. \tag{1.9}$$

Since the time average of a sinusoid (over an integer number of periods) vanishes, and the time average of the square of a sinusoid is 1/2,

$$I = I_0 \frac{1 + \cos\delta}{2}, \tag{1.10}$$

where $I_0 = \mathcal{E}_0^2 \langle \cos^2[\omega t] \rangle = \mathcal{E}_0^2/2$ is the entrance intensity and $\delta = \delta_1 - \delta_2$ is the difference between the reflection phase shifts of the two paths.

Assume there is a phase shift of $\pi/2$ radians at each reflection. (The actual phase shifts depend on the detailed characteristics of the optical elements, but can always be adjusted by inserting dielectric slabs in one or both paths of the interferometer). At the up exit, the difference in phase shifts $\delta = 3(\pi/2) - (\pi/2) = \pi$, and so the intensity $I = 0$. At the right exit, the difference in phase shifts $\delta = 2(\pi/2) - 2(\pi/2) = 0$, and so the intensity $I = I_0$.

1.2.8 Mach-Zehnder Quantum Model 1

Next create a more quantitative quantum model of the Mach-Zehnder interferometer, one that works for faint light, when only single photons are in the interferometer. How can it reproduce wave interference with particles? Adopt a model due to Richard Feynman.

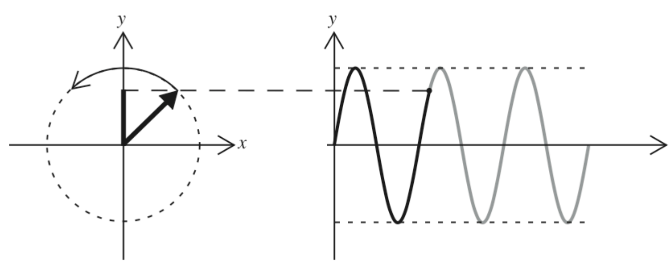


Figure 1.12: Vertical projection (left) of a rotating vector (right) varies sinusoidally.

The projection of a rotating arrow in a fixed direction varies sinusoidally, like a wave train, as in Fig. 1.12. This suggests the following scheme. Imagine that, along each path through the interferometer, a photon carries an arrow that rotates at the frequency of the corresponding classical light. For the purposes of the illustration in Fig. 1.13, assume that each arrow rotates $\pi/4$ radians per step, plus an extra $\pi/2$ radians per reflection, and shortens by $1/\sqrt{2}$ at each beam splitter. At the mirrors and beam splitters, draw the arrow just before in gray and just after in black. Adding the arrows for both paths at the exit and squaring correctly gives the probability of detecting the photon. For bright light, this corresponds to squaring the electric field amplitude to obtain the intensity.

1.2.9 Mach-Zehnder Quantum Model 2

Conveniently and compactly represent the rotating arrows by complex numbers $\rho e^{i\varphi}$ of modulus ρ and argument $\varphi = kz - \omega t$, where z and t are the (real) propagation distance and time, and $\omega/k = c$. For definiteness, assume a $\pi/2$ phase shift upon reflections. Label the states of a photon in each segment of the interferometer using the conventional quantum notation $|\bullet\rangle$, called a *ket*

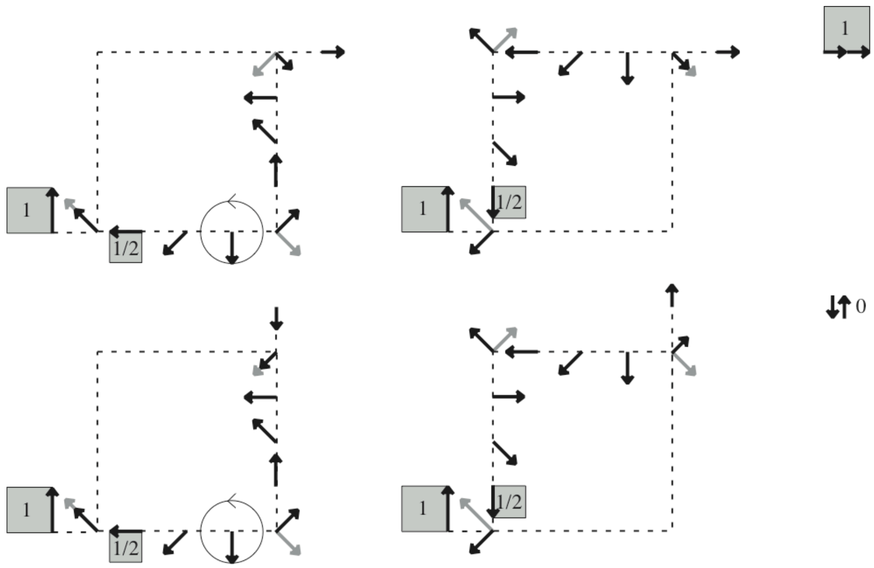


Figure 1.13: A photon carries an imaginary arrow that rotates at the frequency of the corresponding classical light. Adding the arrows at the exit for both paths and squaring gives the probability of detecting the photon: unity for exiting right (top row) and zero for exiting up (bottom row).

(from the word bracket), as in Fig. 1.14. At the first beam splitter, the initial photon state $|a\rangle$ evolves to a *quantum superposition* of a transmitted photon state $|b\rangle$ and a reflected photon state $|c\rangle$. If ℓ is the length of one segment of the interferometer, and the photon is at the first beam splitter at $z = 0$ and $t = 0$, then

$$|a\rangle \longrightarrow \frac{1}{\sqrt{2}} e^{i(k\ell/2-\omega t)} |b\rangle + \frac{1}{\sqrt{2}} e^{i(k\ell/2-\omega t+\pi/2)} |c\rangle . \tag{1.11}$$

The complex numbers multiplying each state record the amplitude and phase of the rotating arrows: the moduli $1/\sqrt{2}$ account for the passage through the beam splitter, while the $\pi/2$ in the argument of the second complex number accounts for the reflection phase shift.

According to the CI, if the experiment were stopped here, and the photon's transmittance or reflectance observed, the square of the moduli of these complex numbers would be the corresponding probabilities

$$\mathcal{P}[b] = \left| \frac{1}{\sqrt{2}} e^{i(k\ell/2-\omega t)} \right|^2 = \frac{1}{2}, \tag{1.12a}$$

$$\mathcal{P}[c] = \left| \frac{1}{\sqrt{2}} e^{i(k\ell/2-\omega t+\pi/2)} \right|^2 = \frac{1}{2}. \tag{1.12b}$$

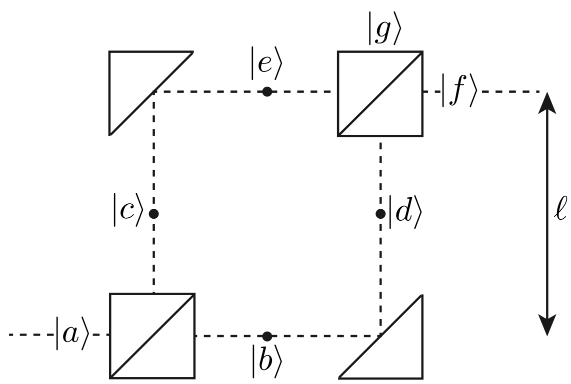


Figure 1.14: Photon states in the interferometer.

According to the MWI, the quotient of these two numbers $\mathcal{P}[b]/\mathcal{P}[c] = 1$ is the branching ratio for the two different histories.

In practice, to calculate the interference only a record of the *difference* in the phases of the two paths is needed. Consequently, abbreviate the effect of the first beam splitter by the evolution

$$|a\rangle \longrightarrow \frac{1}{\sqrt{2}}\,|b\rangle + \frac{i}{\sqrt{2}}\,|c\rangle\,, \tag{1.13}$$

where $i = e^{i\pi/2}$ accounts for the reflection phase shift. Similarly, the mirrors induce

$$|b\rangle \longrightarrow i\,|d\rangle\,, \tag{1.14a}$$

$$|c\rangle \longrightarrow i\,|e\rangle\,, \tag{1.14b}$$

while the second beam splitter induces

$$|d\rangle \longrightarrow \frac{i}{\sqrt{2}}\,|f\rangle + \frac{1}{\sqrt{2}}\,|g\rangle \tag{1.15a}$$

$$|e\rangle \longrightarrow \frac{1}{\sqrt{2}}\,|f\rangle + \frac{i}{\sqrt{2}}\,|g\rangle\,. \tag{1.15b}$$

The complete evolution is

$$|a\rangle \longrightarrow \frac{1}{\sqrt{2}}\left(i\,|d\rangle - |e\rangle\right) = \frac{1}{2}\left(-\,|f\rangle + i\,|g\rangle - |g\rangle - i\,|g\rangle\right) = -\,|f\rangle \tag{1.16}$$

or

$$|a\rangle \longrightarrow -\,|f\rangle + 0\,|g\rangle\,. \tag{1.17}$$

Hence, the probabilities

$$\mathcal{P}[f] = |-1|^2 = 1, \tag{1.18a}$$

$$\mathcal{P}[g] = |\,0\,|^2 = 0, \tag{1.18b}$$

as expected. The certainty of $|f\rangle$ (exiting right) and the impossibility of $|g\rangle$ (exiting up) is an example of *quantum interference*.

1.3 Measurement & Entanglement

Light elucidates the measurement problem and quantum entanglement.

1.3.1 Hilbert Space Preview

In general, if $|\varphi\rangle$ and $|\psi\rangle$ are quantum states, then any linear combination $a|\varphi\rangle + b|\psi\rangle$, with complex coefficients a and b, is also a quantum state. In fact, such states form a *Hilbert space*: a linear vector space with a complex scalar product. For example, the calcite crystal of Section 1.1 can induce a photon to evolve to a state $|\psi\rangle$ that is a superposition of horizontal $|h\rangle$ and vertical $|v\rangle$ polarization, namely

$$|\psi\rangle = a\,|h\rangle + b\,|v\rangle\,, \tag{1.19}$$

where $|a|^2 + |b|^2 = 1$ to conserve probability. (Measurement will certainly find the photon in one of the two states.) The set of all such states form a quantum bit or *qubit*, which is of fundamental importance in quantum computing: while a classical bit can be in one of two states, a qubit can be in an infinite number of superpositions of states.

A quantum superposition is a kind of complex-number-weighted coexistence of possibilities (or potentialities). According to the CI, the absolute square of the weights correspond to the probabilities of measuring the alternatives. According to the MWI, the quotient of the weights is the branching ratio for the two different histories. (The branching ratio must be a rational number, but rationals can approximate real numbers arbitrarily well.)

1.3.2 Quantum Evolution

As shown below, superpositions evolve *continuously* and *deterministically* under the *Schrödinger* differential equation, in both the CI and the MWI. For example,

$$|\psi\rangle \xrightarrow{S} |\psi'\rangle = a'\,|h\rangle + b'\,|v\rangle\,. \tag{1.20}$$

In the CI, but not in the MWI, there is also a *discontinuous* and *probabilistic* collapse of a superposition to classical probability-weighted alternatives when the system is *measured* (or observed or registered). For example,

$$|\psi'\rangle \xrightarrow{M} \left\{ \begin{array}{ll} |h\rangle\,, & \mathcal{P}[h] = |a'|^2 \\ |v\rangle\,, & \mathcal{P}[v] = |b'|^2 \end{array} \right\}. \tag{1.21}$$

While the S-evolution is uncontroversial, the same cannot be said about the M-evolution.

1.3.3 Schrödinger's Cat and the Measurement Problem

Consider a variation of the (in)famous Schrödinger cat experiment, wherein a (working) bomb amplifies a microscopic superposition to macroscopic proportions, as in Fig. 1.15, where a single photon interacts with a beam splitter. In the absence of a measurement, the system $|\psi\rangle$ evolves into a superposition of reflected and transmitted photons

$$|\psi\rangle \xrightarrow{S} |\psi'\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\rightarrow\rangle\,, \tag{1.22}$$

and unexploded and exploded bombs

$$|\psi'\rangle \xrightarrow{S} |\psi''\rangle = \frac{1}{\sqrt{2}}|\uparrow, \bullet\rangle + \frac{1}{\sqrt{2}}|\rightarrow, \star\rangle \tag{1.23}$$

and calm and distressed observers

$$|\psi''\rangle \xrightarrow{S} |\psi'''\rangle = \frac{1}{\sqrt{2}}|\uparrow, \bullet, ☺\rangle + \frac{1}{\sqrt{2}}|\rightarrow, \star, ☹\rangle\,. \tag{1.24}$$

Such macroscopic superpositions are called *Schrödinger cat states.* (In the original thought experiment, the observer was a cat.) However, superpositions of unexploded and exploded bombs are not observed, nor of calm and distressed people, whatever that might mean. According to the CI, to *collapse* the superposition

$$|\psi'''\rangle \xrightarrow{M} \left\{ \begin{array}{ll} |\uparrow, \bullet, ☺\rangle\,, & \mathcal{P} = \left|1/\sqrt{2}\right|^2 = 1/2 \\ |\rightarrow, \star, ☹\rangle\,, & \mathcal{P} = \left|1/\sqrt{2}\right|^2 = 1/2 \end{array} \right\}, \tag{1.25}$$

a measurement must occur at the beam splitter, or at the bomb, or at the observer, or ... .

But exactly where and when does the superposition collapse? Are not the beam splitter, the bomb, and the observer all ultimately quantum systems? Where is the threshold between microscopic and macroscopic, between experiment and experimenter, between phenomenon and observer, between quantum and classical? Physicist Eugene Wigner argued that the threshold is human consciousness. The chief architect of the CI, Neils Bohr, argued that the threshold is *relative*; it depends on one's point of view, on how one chooses to analyze the experiment, so there is no one right answer to where and when the superposition's complex-number-weighted coexistence of multiple possibilities collapses into a probability-weighted single reality.

The MWI dispenses with this so-called "measurement" problem by entirely eliminating the discontinuous, probabilistic M-evolution. According to the MWI, two histories continuously and deterministically emerge from the experiment, one including a calm observer, an unexploded bomb, and a reflected photon, the other including a distressed observer, an exploded bomb, and a transmitted photon. The apparent probabilities and discontinuities are merely artifacts of individual observers being confined to single histories.

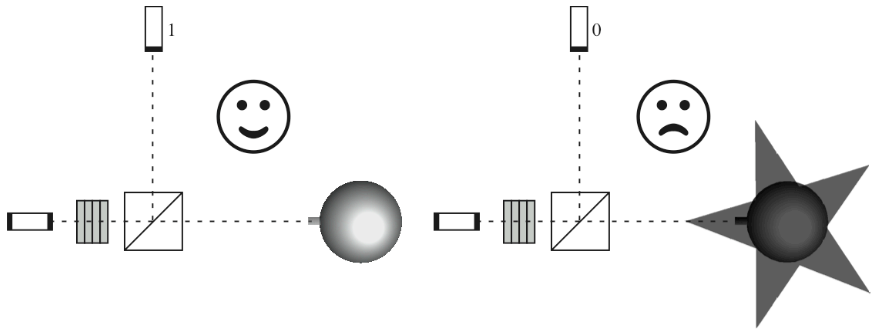


Figure 1.15: Single photon incident on a beam splitter is reflected and detected by a PMT, calming the observer (left), or is transmitted and detonates a bomb, distressing the observer (right). The $\mathcal{S}$-evolution places the photon, the bomb, and the observer in a macroscopic quantum superposition, a Schrödinger cat state.

1.3.4 Polarization

Beam splitters and mirrors control the *direction* of classical light and the *linear momenta* of photons. Calcite crystals, quarter wave plates, and polarizers control the *polarization* of classical light and the *angular momenta* (or *spin*) of photons. This latter capability facilitates investigation of additional aspects of quantum reality.

In classical optics, polarization refers to the oscillation of the light's electric field. If light is traveling in the z-direction at speed $c = \omega/k$, then

$$\vec{\mathcal{E}}_h[\delta_h] = \hat{x}\,\mathcal{E}_0 \cos[kz - \omega t + \delta_h], \tag{1.26a}$$

$$\vec{\mathcal{E}}_v[\delta_v] = \hat{y}\,\mathcal{E}_0 \cos[kz - \omega t + \delta_v]\,, \tag{1.26b}$$

represent horizontal and vertical *linearly polarized* light, because the electric field is oscillating in a line. Superpose this light with different relative phases $\delta_h - \delta_v$ to create differently polarized light. For example, if the relative phase shift is zero, then

$$\vec{\mathcal{E}}_d = \vec{\mathcal{E}}_b[0] + \vec{\mathcal{E}}_v[0] = (\hat{x} + \hat{y})\,\mathcal{E}_0 \cos[kz - \omega t]\,, \tag{1.27}$$

represents diagonally polarized light, which is just linearly polarized light in a different direction. If the relative phase shift is $\pm\pi/2$, then

$$\vec{\mathcal{E}}_r = \vec{\mathcal{E}}_h[0] + \vec{\mathcal{E}}_v[+\pi/2] = (\hat{x}\cos[kz - \omega t] - \hat{y}\sin[kz - \omega t])\,\mathcal{E}_0, \tag{1.28a}$$

$$\vec{\mathcal{E}}_\ell = \vec{\mathcal{E}}_h[0] + \vec{\mathcal{E}}_v[-\pi/2] = (\hat{x}\cos[kz - \omega t] + \hat{y}\sin[kz - \omega t])\,\mathcal{E}_0, \tag{1.28b}$$

represent right hand and left hand *circularly polarized* light, because the electric field rotates in a circle at each place in space. In the particle physics convention, at each place, right hand light rotates as the right hand fingers curl when the right thumb points in the propagation direction. The corresponding relations for photons correspond to the classical relations for light waves. A "diagonal" photon is a superposition

$$|d\rangle = \frac{1}{\sqrt{2}}|h\rangle + \frac{1}{\sqrt{2}}|v\rangle . \tag{1.29}$$

"Circular" or natural photons are the superpositions

$$|r\rangle = \frac{1}{\sqrt{2}}|h\rangle + \frac{i}{\sqrt{2}}|v\rangle , \tag{1.30a}$$

$$|\ell\rangle = \frac{1}{\sqrt{2}}|h\rangle - \frac{i}{\sqrt{2}}|v\rangle , \tag{1.30b}$$

where the $\pm i = e^{\pm i\pi/2}$ account for the relative phase shifts. Since photons are naturally circular, it is appropriate to invert these relations and write

$$|h\rangle = \frac{1}{\sqrt{2}}\left(|r\rangle + |\ell\rangle\right) , \tag{1.31a}$$

$$|v\rangle = \frac{-i}{\sqrt{2}}\left(|r\rangle - |\ell\rangle\right) . \tag{1.31b}$$

In a measurement of the linear polarization of $|v\rangle$, $|r\rangle$ and $|\ell\rangle$ are equally likely,

$$|v\rangle \xrightarrow{M} \left\{ \begin{array}{ll} |r\rangle , & \mathcal{P} = \left|-i/\sqrt{2}\right|^2 = 1/2 \\ |\ell\rangle , & \mathcal{P} = \left|+i/\sqrt{2}\right|^2 = 1/2 \end{array} \right\} , \tag{1.32}$$

but the complex numbers $\pm i$ are crucial to recovering $|r\rangle$ when superposing $|h\rangle$ and $|v\rangle$, as in Eq. 1.30a.

Measuring the linear polarization of a photon places it in a superposition of right and left circular polarizations, while measuring the circular polarization places the photon in a superposition of linear polarizations. In fact, a photon cannot have both linear and circular polarization simultaneously; knowing one type of polarization leaves the other type *indeterminate*, a special case of the *Heisenberg indeterminacy principle*.

Optically anisotropic materials with different indices of refraction in different directions can transform light from one polarization to another. A calcite crystal can convert a diagonal light beam into parallel beams of horizontal and vertical light. A *quarter wave plate* can convert diagonal light into circular light (by retarding one component by a distance $\lambda/4$).

1.3.5 Crossed Polarizers

An ideal polarizer converts unpolarized light into linearly polarized light by selectively transmitting only one polarization. Consider light traveling in the z-direction, and linearly polarized in the x-direction, incident on a polarizer with transmission axis an angle θ from the x-direction, as in Figure 1.16. If the transmission direction is x' and the perpendicular direction is y', then decompose the incident electric field amplitude as the superposition

$$\vec{\mathcal{E}}_0 = \hat{x}'\mathcal{E}_0 \cos\theta + \hat{y}'\mathcal{E}_0 \sin\theta. \tag{1.33}$$

Therefore, the transmitted amplitude is

$$\mathcal{E}_0' = \mathcal{E}_0 \cos\theta \tag{1.34}$$

and, since intensity is proportional to the amplitude squared, the transmitted intensity is

$$I' = I\cos^2\theta, \tag{1.35}$$

which is *Malus's Law.*

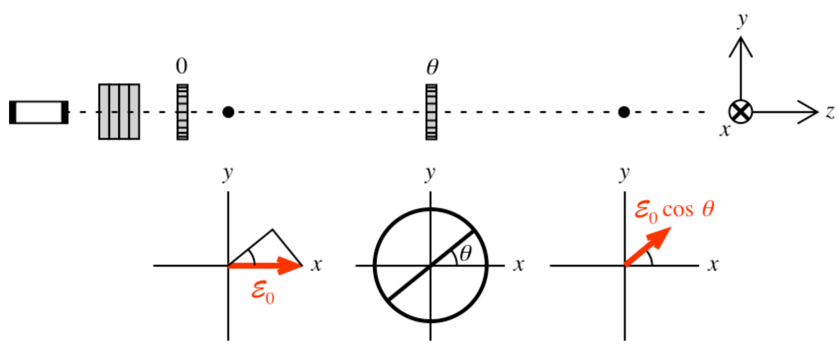


Figure 1.16: A polarizer transmits the component of light parallel to its transmission axis.

Similarly, a photon polarized in the x-direction is a superposition of a photon polarized in the parallel and perpendicular directions,

$$|x\rangle = \cos\theta\,|x'\rangle + \sin\theta\,|y'\rangle\,. \tag{1.36}$$

Therefore

$$|x\rangle \xrightarrow{M} \left\{ \begin{array}{ll} |x'\rangle\,, & \mathcal{P} = |\cos\theta|^2 = \cos^2\theta \\ |y'\rangle\,, & \mathcal{P} = |\sin\theta|^2 = \sin^2\theta \end{array} \right\}, \tag{1.37}$$

and hence the probability of transmission is $\cos^2\theta$, which corresponds to Malus's law.

Consider next a single photon incident on crossed polarizers, as in Fig. 1.17. If the probability of transmission at the first polarizer is 1/2 and the probability of transmission at the second polarizer is $\cos^2\theta$, then the probability of transmission through both polarizers is $(1/2)\cos^2\theta$. If the relative angle between the two transmission axes is $\theta = \pi/2$, then no photons get through. However,

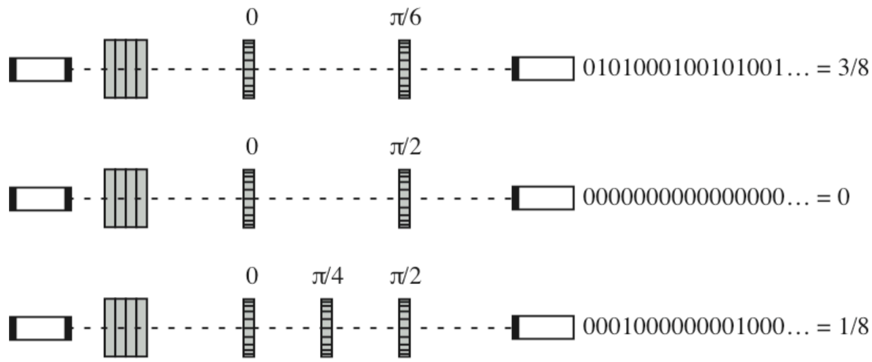


Figure 1.17: Single photon incident on crossed polarizers. Transmission probabilities correspond to Malus's law.

inserting a third polarizer between the previous two with transmission axis at $\theta = \pi/4$ causes one in eight photons gets through — *adding* an intermediate polarizer has *increased* the probability of transmission! These faint light, quantum experiments correspond well to the analogous bright light, classical experiments.

1.3.6 Entangled States

Pairs of quantum particles can be *entangled* so that a property of one, such as its polarization (spin), is linked intimately with that of the other. Such entangled or "twinned" pairs of particles are *superpositions* of states.

Consider *positronium*, a bound state of an electron e^- and its antiparticle, the positron e^+. Its ground state has zero angular momentum and odd (negative) *parity*. It is unstable and decays after about 10^{-10} s into a pair of entangled photons, as in Fig. 1.18. To conserve linear momentum, the photons must have equal but opposite momenta. To conserve angular momentum, the spin of the photons must also be equal but opposite, implying identical circular polarization. To conserve parity, these two indistinguishable alternatives must superpose with a minus sign to form the entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\,|r\rangle\,|r\rangle - \frac{1}{\sqrt{2}}\,|\ell\rangle\,|\ell\rangle = \frac{1}{\sqrt{2}}\left(|rr\rangle - |\ell\ell\rangle\right). \tag{1.38}$$

(Parity refers to the behavior of a system under coordinate inversion. If P is the parity operator, then $P|rr\rangle = |\ell\ell\rangle$ and $P|\ell\ell\rangle = |rr\rangle$, and so $P|\psi\rangle = -|\psi\rangle$.)

Although photons correspond to circular rather than linear light, they can be analyzed into completely anticorrelated plane polarizations. Using Eq. 1.30 to express circular polarizations as superpositions of linear polarizations, the entangled state becomes

$$|\psi\rangle = \frac{i}{\sqrt{2}}\,|h\rangle\,|v\rangle + \frac{i}{\sqrt{2}}\,|v\rangle\,|h\rangle = \frac{i}{\sqrt{2}}\left(|hv\rangle + |vh\rangle\right). \tag{1.39}$$

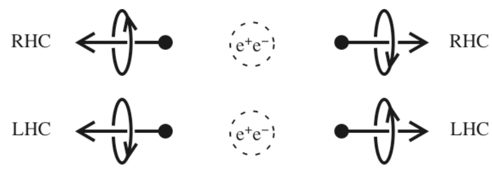


Figure 1.18: Positronium (top) annihilates into a pair of right circular photons (middle) or a pair of left circular photons (bottom). Both possibilities superpose to form an entangled state. The photon emission is isotropic.

Any linear polarization measurement induces a nonlocal collapse of the superposition

$$|\psi\rangle \xrightarrow{M} \left\{ \begin{array}{ll} |hv\rangle\,, & \mathcal{P} = \left|i/\sqrt{2}\right|^2 = 1/2 \\ |vh\rangle\,, & \mathcal{P} = \left|i/\sqrt{2}\right|^2 = 1/2 \end{array} \right\}, \tag{1.40}$$

at least in the CI. After the measurement, one photon is horizontally polarized and the other is vertically polarized.

1.3.7 EPR-Bohm Experiment

Consider an experiment first proposed in the 1930s by Albert Einstein, Boris Podolsky, and Nathan Rosen (EPR) [9] and modernized in the 1950s by David Bohm. Suppose two observers, Alice and Bob, intercept entangled photons with linear polarizers at a relative angle of θ, as in Fig. 1.19. For each photon pair, the two polarization measurements can be separated by a spacelike interval, so far apart that not even light can join them. Each measurement can be reduced to a binary digit, 1 or 0, indicating a photon transmitted or not. Alice and Bob's binary data for many measurements imply the *correlation function*

$$C[\theta] = \frac{\#\text{matches}}{\#\text{trials}} = \mathcal{P}[\text{match}]. \tag{1.41}$$

For $\theta = 0$, Alice and Bob's data are sequences of random digits, with 0 and 1 equally likely, but perfectly *anticorrelated*, in agreement with Eq. 1.40, so that $C[0] = 0$. For $\theta = \pi/2$, Alice and Bob's data are other sequences of random digits, but now perfectly *correlated*, again in agreement with Eq. 1.40, so that $C[\pi/2] = 1$. To calculate the quantum prediction for the correlation function at an arbitrary angle, begin with basic probability theory. If the conventional symbols $\wedge$, $\vee$, $|$, denote "and", "or", "given", then

$$\begin{aligned} \mathcal{P}[\text{match}] &= \mathcal{P}[(A=0 \wedge B=0) \vee (A=1 \wedge B=1)], && (1.42a)\\ &= \mathcal{P}[A=0]\mathcal{P}[B=0|A=0] + \mathcal{P}[A=1]\mathcal{P}[B=1|A=1], && (1.42b)\\ &= \mathcal{P}[A=0]\,(1-\mathcal{P}[B=1|A=0]) + \mathcal{P}[A=1]\mathcal{P}[B=1|A=1]. && (1.42c) \end{aligned}$$

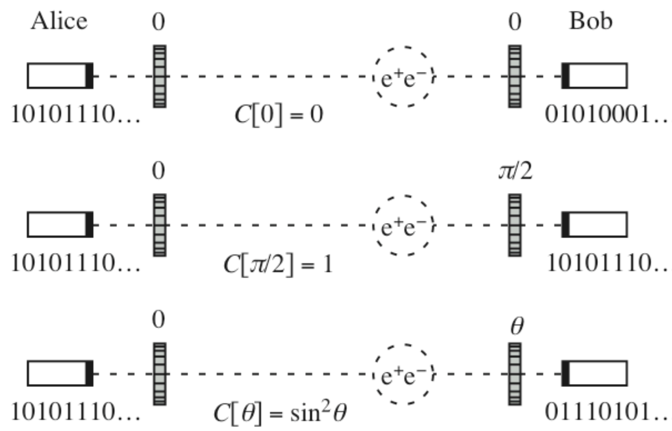


Figure 1.19: Polarization cross correlations of entangled photon pairs.

The Section 1.3.5 Malus's law results and the identity $C[\theta] = \mathcal{P}[\text{match}]$ imply

$$C[\theta] = \frac{1}{2}\left(1 - \cos^2\theta\right) + \frac{1}{2}\cos^2\left[\frac{\pi}{2} - \theta\right] \tag{1.43}$$

or

$$C[\theta] = \sin^2\theta, \tag{1.44}$$

which agrees with the extreme cases $C[0] = 0$ and $C[\pi/2] = 1$. For small nonzero angles, $\sin\theta \sim \theta \ll 1$ and $C[\theta] \sim \theta^2$, so $C[2\theta] \sim 4\theta^2 > 2\theta^2 = 2C[\theta]$, or

$$C[2\theta] > 2C[\theta]. \tag{1.45}$$

1.3.8 Bell's Inequality

In 1964, John Bell demonstrated [10] that any classical (local realistic) explanation for an EPR-Bohm-type experiment must produce weaker correlations. To show this, if Alice and Bob's polarizer are aligned, so that their relative angle $\theta = 0$, then their binary data are completely anticorrelated, $C[0] = 0$. If Bob now rotates his polarizer through an angle $\theta > 0$, the misalignment introduces some matches into his data (by, say, flipping a 1 to a 0), so $C[\theta] > 0$. If Alice next rotates her polarizer through the same angle, the realignment removes the matches from her data (by flipping a 1 to a 0), so again $C[0] = 0$. If Bob next rotates his polarizer through an additional angle $\theta > 0$, the second misalignment once more introduces some matches into his data, so again $C[\theta] > 0$. However, if Alice had not rotated her polarizer, the successive misalignments of Bob's polarizer might have cancelled some matches (by flipping a 0 to a 1 and then back to a 0 again). Hence

$$C[2\theta] \leq 2C[\theta], \tag{1.46}$$

which is an example of a Bell inequality.

The quantum prediction of Eq. 1.45 contradicts the classical prediction of Eq. 1.46, so put nature to the test. By the 1980s, in a culmination of a series of increasingly better experiments by many research groups, Alain Aspect and colleagues convincingly demonstrated that Bell's inequality is decisively violated in these kind of experiments. Consequently, there must be something wrong with Bell's argument, as Bell himself anticipated.

The argument seems to rest on two assumptions: locality and reality. *Locality* means no superluminal connections, so what happens here and now doesn't depend on what happens then and there. For example, the argument implicitly assumes locality when it reasons that, when Bob rotates his polarizer, he alters his data but not Alice's, and vice versa. Reality means *counterfactual definiteness*, the ability to consistently discuss what might have happened but did not. For example, the argument reasons that if Bob *had* rotated his polarizer through θ, then he *would have* introduced some matches, and if he *had then* rotated through an additional θ, then some of the matches *might have* cancelled. One of these two classically reasonable assumptions must be wrong.

A popular nonlocal interpretation of the EPR-Bohm experiment is that it is impossible to force a two-particle interpretation on an entangled particle pair. While this may violate the spirit of special relativity, it does not violate the letter of special relativity. In the CI, quantum randomness prevents using entangled states for *superluminal telegraphs*, because any message introduced by rotating one of the polarizers is found only in the correlations between possibly remote and spacelike experiments. In the MWI, measurements don't collapse superpositions, nonlocally or otherwise, and locality is restored.

Problems

1. Complex numbers are used extensively in quantum physics. Common notations are

$$z = x + iy = r(\cos\theta + i\sin\theta) = re^{i\theta}, \tag{1.47}$$

and a fundamental operation is complex conjugation

$$z^* = \bar{z} = x - iy = r(\cos\theta - i\sin\theta) = re^{-i\theta}, \tag{1.48}$$

where $i = \sqrt{-1}$. Find the principal values of the following numbers in the form $x + iy$, where $x, y \in \mathcal{R}$ are real numbers.

   (a) $\dfrac{1}{1+i}$.

   (b) $25e^{2i}$ (Caution: The angle is 2 radians *not* 2π radians.)

   (c) $\dfrac{3i-7}{i+4}$ (Caution: The numerator is *not* $3-7i$.)

   (d) $\left(\dfrac{1+i}{1-i}\right)^{2718}$ (Hint: Don't use a calculator or computer!)

   (e) $\sqrt{i}$

   (f) i^i

2. Prove the following equations.

   (a) $e^{i\theta} = \cos\theta + i\sin\theta$ (Hint: Use Taylor series expansions.)

   (b) $e^{i\pi} + 1 = 0$ (Euler's tombstone.)

   (c) $\sin\theta = \dfrac{e^{i\theta} - e^{-i\theta}}{2i}$

   (d) $\cos\theta = \dfrac{e^{i\theta} + e^{-i\theta}}{2}$

3. **Malus's law and the inverse quantum Zeno effect.** Consider a sequence of $N+1$ polarizers each rotated at an angle $\pi/2N$ relative to its neighbors. Suppose a photon passes through the first polarizer.

   (a) What is the probability that it passes through the second polarizer? (Hint: Consult Eq. 1.37.)

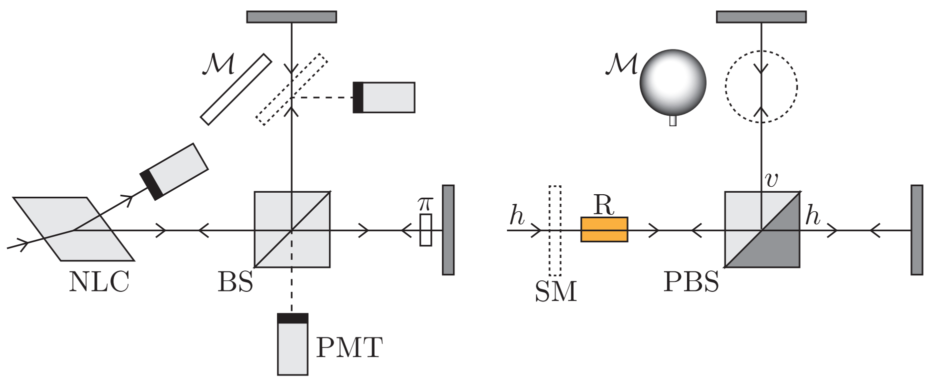
   (b) What is the probability that it passes through all the rest of the polarizers?

   (c) Show that the probability of transmission increases to unity as the number of polarizers increases to infinity. Thus, a dense set of "measurements" can rotate the photon's plane of polarization through a right angle!

4. **Experimental interaction-free measurements.** A nonlinear optical crystal down-converts a UV laser photon to a pair of low-energy photons traveling 30° from each other. The detection of one confirms the existence of the other, which is directed into a Michelson interferometer (left below). Without the "Medusa" mirror in the interferometer's orthogonal path, virtually all photons exit the way they came, with virtually no photons exiting down, due to destructive interference.

   (a) With the Medusa mirror in place, what fraction of photons exit down, thereby registering the Medusa without seeing it?

   (b) By reducing the beam splitter's reflection probability $p \ll 1/2$, what fraction of measurements can be made interaction-free? (Hint: Exclude cases where a photon exits the way it enters.)



5. **Improved null measurements.** This interferometer (right above) exploits the inverse quantum Zeno effect. Time the switchable mirror to allow the photon to go back-and-forth through the system N times. Sugar water rotates the polarization plane $\pi/4N$ each time the photon passes through it. The time-reversible polarizing beam splitter sends horizontally and vertically polarized light in orthogonal directions. Input photons are horizontally polarized.

   (a) By how much does the sugar water rotate the polarization when the photon pass back *and* forth through it?

   (b) When the vertical path is clear of the "Medusa" bomb, why does the photon exit the system vertically polarized?

   (c) When the Medusa blocks the vertical path, why does the photon exit nearly horizontally polarized (when it isn't absorbed) for large N?

   (d) Now quantitatively, with what probability does the Medusa *not* absorb the photon when it blocks the vertical path?

   (e) Consequently, what fraction of measurements are interaction-free as $N \to \infty$?

6. **Photon Polarization.** First consider classic light propagating in the z-direction.

   (a) Show that

$$\vec{\mathcal{E}}_R = \mathcal{E}_0(\hat{x}\cos[kz-\omega t] + \hat{y}\cos[kz-\omega t+\pi/2]), \tag{1.49a}$$
$$\vec{\mathcal{E}}_L = \mathcal{E}_0(\hat{x}\cos[kz-\omega t] + \hat{y}\cos[kz-\omega t-\pi/2]), \tag{1.49b}$$

   represent right and left circularly polarized light. Hint: Sketch the rotation of the electric fields at a fixed point in space.

   (b) Show that

$$\vec{\mathcal{E}}_x = \vec{\mathcal{E}}_L + \vec{\mathcal{E}}_R, \tag{1.50a}$$
$$\vec{\mathcal{E}}_y = \vec{\mathcal{E}}_L - \vec{\mathcal{E}}_R, \tag{1.50b}$$

   represent linear polarized light.

   (c) Express circular light as linear superpositions of linear light.

   (d) In order to correspond with classical light, assume that circularly polarized photons are superpositions of linearly polarized photons and their states are related by

$$|r\rangle = \frac{1}{\sqrt{2}}|x\rangle + \frac{1}{\sqrt{2}}e^{+i\pi/2}|y\rangle, \tag{1.51a}$$
$$|\ell\rangle = \frac{1}{\sqrt{2}}|x\rangle + \frac{1}{\sqrt{2}}e^{-i\pi/2}|y\rangle. \tag{1.51b}$$

   Show that

$$|x\rangle = \frac{1}{\sqrt{2}}|\ell\rangle + \frac{1}{\sqrt{2}}|r\rangle, \tag{1.52a}$$
$$|y\rangle = \frac{i}{\sqrt{2}}|\ell\rangle - \frac{i}{\sqrt{2}}|r\rangle. \tag{1.52b}$$

   (e) Rotate the coordinate system through an angle φ in the xy-plane. Justify

$$|x'\rangle = +\cos\varphi|x\rangle + \sin\varphi|y\rangle, \tag{1.53a}$$
$$|y'\rangle = -\sin\varphi|x\rangle + \cos\varphi|y\rangle. \tag{1.53b}$$

   (f) Show that the rotated circular polarizations satisfy

$$|r'\rangle = e^{-i\varphi}|r\rangle, \tag{1.54a}$$
$$|\ell'\rangle = e^{+i\varphi}|\ell\rangle. \tag{1.54b}$$

   (g) Show then that the probability of measuring a circularly polarized photon to have a particular linear polarization is the same at any angle. Why is this so physically?

7. Create a single photon model of the Fig. 1.9 quantum eraser. Assume an initial diagonal polarization state $|D\rangle = (|h\rangle + |v\rangle)/\sqrt{2}$. The effect of the vertical polarizer is $|\psi\rangle \rightarrow |v\rangle\langle v|\psi\rangle$, where the complex "bra-ket" scalar products $\langle v|v\rangle = 1$ and $\langle h|v\rangle^* = \langle v|h\rangle = 0$, for example. Generalizing Section 1.2.9, track both location *and* polarization by working in the product Hilbert space $|LP\rangle = |L\rangle|P\rangle \in \mathcal{H}_L \otimes \mathcal{H}_P$, where $\langle Lh|L'v\rangle = \langle L|L'\rangle\langle h|v\rangle = 0$, for example. Track phase shifts by modeling the beam splitter with transmission and reflection coefficients $t = 1/\sqrt{2}$ and $r = i/\sqrt{2}$.

   (a) Compute the probabilities for the photon to exit up and right with the analyzers horizontal.

   (b) Compute the probabilities for the photon to exit up and right with the analyzers diagonal.

Chapter 2

Hilbert Spaces

Generalize Euclidean space to mathematically describe quantum phenomena.

2.1 Euclidean Space

The familiar real scalar product defines distances and angles. Completeness (the inclusion of all limited points) makes possible calculus. If places

$$\vec{u}, \vec{v}, \vec{w} \in \mathcal{R}^3 \tag{2.1}$$

and real coefficients

$$a, b, c \in \mathcal{R}, \tag{2.2}$$

then the linear superposition

$$a\vec{u} + b\vec{v} + c\vec{w} \in \mathcal{R}^3. \tag{2.3}$$

is also a place. Use the real and symmetric scalar or dot product

$$\vec{u} \cdot \vec{v} = \vec{v} \cdot \vec{u} \in \mathcal{R} \tag{2.4}$$

to define an orthonormal basis

$$\hat{x}_m \cdot \hat{x}_n = \hat{m} \cdot \hat{n} = \delta_{mn}. \tag{2.5}$$

Decompose a vector

$$\vec{v} = v_1 \hat{x}_1 + v_2 \hat{x}_2 + v_3 \hat{x}_3 = \sum_n v_n \hat{x}_n = \sum_n \hat{x}_n v_n, \tag{2.6}$$

where the projections

$$v_n = \hat{x}_n \cdot \vec{v} \in \mathcal{R} \tag{2.7}$$

imply

$$\vec{v} = \hat{x}_1(\hat{x}_1 \cdot \vec{v}) + \hat{x}_2(\hat{x}_2 \cdot \vec{v}) + \hat{x}_3(\hat{x}_3 \cdot \vec{v}) = \sum_n \hat{x}_n \left(\hat{x}_n \cdot \vec{v}\right) \tag{2.8}$$

and

$$v^2 = \vec{v} \cdot \vec{v} = \sum_n \left(\hat{x}_n \cdot \vec{v}\right)\left(\hat{x}_n \cdot \vec{v}\right) = \sum_n \left(\hat{x}_n \cdot \vec{v}\right)^2 = \sum_n v_n^2. \tag{2.9}$$

2.2 Generic Hilbert Space

2.2.1 Vectors

To describe quantum phenomena requires more general n-dimensional Hilbert spaces $\mathcal{H}$ equipped with *complex* scalar products. (If $x, y \in \mathcal{R}$ are real numbers and $i = \sqrt{-1}$, then $z = x + iy \in \mathcal{C}$ is a complex number, and $z^* = \bar{z} = x - iy$ is its *complex conjugate*.) In conventional Dirac bra(c)ket notation, if states

$$|\varphi\rangle, |\chi\rangle, |\psi\rangle \in \mathcal{H}, \tag{2.10}$$

(pronounced "ket phi, ket chi, ket psi") and complex coefficients

$$a, b, c \in \mathcal{C}, \tag{2.11}$$

then the linear superposition

$$a|\varphi\rangle + b|\chi\rangle + c|\psi\rangle \in \mathcal{H} \tag{2.12}$$

is also a state. Use the complex symmetric scalar product

$$\langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^* \in \mathcal{C} \tag{2.13}$$

(pronounced "bra phi ket psi equals bra psi ket phi star") to define an orthonormal basis

$$\langle\psi_m|\psi_n\rangle = \langle m|n\rangle = \delta_{mn}, \tag{2.14}$$

where the *Kronecker delta*

$$\delta_{mn} = \left\{ \begin{array}{ll} 1 & : m = n \\ 0 & : m \neq n \end{array} \right\}. \tag{2.15}$$

Decompose a state

$$|\psi\rangle = \psi_1|1\rangle + \psi_2|2\rangle + \cdots = \sum_n \psi_n|n\rangle = \sum_n |n\rangle\psi_n, \tag{2.16}$$

where the projections

$$\psi_n = \langle n|\psi\rangle \in \mathcal{C} \tag{2.17}$$

imply

$$|\psi\rangle = |1\rangle\langle 1|\psi\rangle + |2\rangle\langle 2|\psi\rangle + \cdots = \sum_n |n\rangle\langle n|\psi\rangle. \tag{2.18}$$

and

$$\langle\psi|\psi\rangle = \sum_n \langle\psi|n\rangle\langle n|\psi\rangle = \sum_n \langle n|\psi\rangle^*\langle n|\psi\rangle = \sum_n |\langle n|\psi\rangle|^2 = \sum_n |\psi_n|^2. \tag{2.19}$$

Among other advantages, the bra ket notation makes it easy to label states without needing to miniaturize the text in a subscript; for example,

$$|0\rangle = |\psi_0\rangle = |\text{ground state}\rangle. \tag{2.20}$$

2.2.2 Operators

In the Hilbert spaces $\mathcal{H}$, scalar products map vectors to numbers, and operators map vectors to vectors. If operators

$$A, B, C \in L[\mathcal{H}], \tag{2.21}$$

then they linearly

$$A\left(a|\varphi\rangle + b|\chi\rangle + c|\psi\rangle\right) = aA|\varphi\rangle + bA|\chi\rangle + cA|\psi\rangle \tag{2.22}$$

map vectors to other vectors

$$A|\psi\rangle = |\psi'\rangle, \tag{2.23}$$

or vectors to multiples of vectors

$$A|\psi_a\rangle = a|\psi_a\rangle, \tag{2.24}$$

which can be abbreviated as

$$A|a\rangle = a|a\rangle, \tag{2.25}$$

where $|a\rangle \in \mathcal{H}$ is an *eigenvector* or *eigenstate* of A and $a \in \mathcal{C}$ is the corresponding *eigenvalue* or *eigenscalar*. The set of all eigenvalues $\{a\}$ of A is the *spectrum* of A.

2.2.3 Dual Space

In a countable Hilbert space, every ket $|\psi\rangle \in \mathcal{H}$ corresponds to a bra in the *dual space*, $|\psi\rangle^\dagger = \langle\psi| \in \mathcal{H}^*$ (pronounced "ket psi dagger equals bra psi in h star"). Every operator A that maps kets to kets

$$|\psi\rangle \underset{A}{\longrightarrow} |\psi'\rangle = A|\psi\rangle \in \mathcal{H} \tag{2.26}$$

corresponds to an *adjoint* operator $A^\dagger$ that maps bras to bras

$$\langle\psi| \underset{A^\dagger}{\longrightarrow} \langle\psi'| = \langle\psi|A^\dagger \in \mathcal{H}^*. \tag{2.27}$$

The adjoint reverses the order of operations. For example, if

$$|\chi\rangle \equiv B|\varphi\rangle, \tag{2.28}$$

then

$$|\psi\rangle \equiv AB|\varphi\rangle = A|\chi\rangle \tag{2.29}$$

so

$$\langle\psi| = \langle\varphi|(AB)^\dagger = \langle\chi|A^\dagger = \langle\varphi|B^\dagger A^\dagger \tag{2.30}$$

and

$$(AB)^\dagger = B^\dagger A^\dagger. \tag{2.31}$$

The adjoint generalized complex conjugation. For example, the adjoint of a complex number

$$c^\dagger = \langle\psi|\varphi\rangle^\dagger = |\varphi\rangle^\dagger\langle\psi|^\dagger = \langle\varphi|\psi\rangle = \langle\psi|\varphi\rangle^* = c^*, \tag{2.32}$$

using the Eq. 2.13 complex symmetry. Furthermore

$$\langle\psi|A|\varphi\rangle^* = \langle\psi|A|\varphi\rangle^\dagger = |\varphi\rangle^\dagger A^\dagger\langle\psi|^\dagger = \langle\varphi|A^\dagger|\psi\rangle. \tag{2.33}$$

For base states $|m\rangle$, the *matrix elements*

$$(A^\dagger)_{mn} = \langle m|A^\dagger|n\rangle = \langle n|A|m\rangle^* = A^*_{nm}. \tag{2.34}$$

To adjoint an expression, reverse the order of the factors (although numbers commute with everything), interchange kets and bras, replace operators by their adjoints and numbers by their complex conjugates.

2.2.4 Hermitian Operators

In a countable Hilbert space, Hermitian operators are *self-adjoint*, so

$$H^\dagger = H. \tag{2.35}$$

Hermitian operators have real eigenvalues and orthogonal eigenstates.

If

$$H|h\rangle = h|h\rangle, \tag{2.36}$$

then

$$\langle h|H = h^*\langle h| \tag{2.37}$$

implies via projection

$$\langle h|H|h\rangle = h\langle h|h\rangle \tag{2.38}$$

and

$$\langle h|H|h\rangle = h^*\langle h|h\rangle. \tag{2.39}$$

The difference

$$0 = (h - h^*)\langle h|h\rangle \tag{2.40}$$

implies the eigenvalue

$$h = h^* \tag{2.41}$$

is real.

If there are two distinct eigenvalues, $h_1 \neq h_2 \in \mathcal{C}$,

$$H|1\rangle = h_1|1\rangle, \tag{2.42a}$$
$$H|2\rangle = h_2|2\rangle, \tag{2.42b}$$

then projection implies

$$\langle 2|H|1\rangle = h_1\langle 2|1\rangle \tag{2.43}$$

and

$$\langle 1|H|2\rangle = h_2\langle 1|2\rangle, \tag{2.44a}$$
$$\langle 1|H|2\rangle^* = (h_2\langle 1|2\rangle)^*, \tag{2.44b}$$
$$\langle 2|H^\dagger|1\rangle = h_2^*\langle 2|1\rangle, \tag{2.44c}$$
$$\langle 2|H|1\rangle = h_2\langle 2|1\rangle. \tag{2.44d}$$

The difference

$$0 = (h_1 - h_2)\langle 2|1\rangle \tag{2.45}$$

implies the eigenstates

$$\langle 2|1\rangle = 0 \tag{2.46}$$

are orthogonal.

2.2.5 Unitary Operators

The adjoint of a unitary operator is its inverse,

$$U^\dagger = U^{-1}, \tag{2.47}$$

so

$$U^\dagger U = I = UU^\dagger, \tag{2.48}$$

where I is the identity operator. Unitary operators have unit eigenvalues and preserve scalar products.

If

$$U|u\rangle = u|u\rangle, \tag{2.49}$$

then

$$\langle u|U^\dagger = \langle u|u^* = u^*\langle u|. \tag{2.50}$$

The product

$$\langle u|u\rangle = \langle u|I|u\rangle = \langle u|U^\dagger U|u\rangle = u^*u\langle u|u\rangle. \tag{2.51}$$

implies

$$1 = |u|^2, \tag{2.52}$$

so the eigenvalue is a *phase factor*, $u = e^{i\varphi}$, where $\varphi \in \mathcal{R}$. In fact, if H is a Hermitian operator, then

$$U = e^{iH} \equiv I + iH - \frac{1}{2}H^2 - i\frac{1}{3!}H^3 + \cdots \tag{2.53}$$

is a unitary operator, where the infinite series expansion defines the exponential of an operator. The adjoint

$$U^\dagger = e^{-iH^\dagger} = e^{-iH} = I - iH - \frac{1}{2}H^2 + i\frac{1}{3!}H^3 + \cdots, \tag{2.54}$$

and because $-iH$ and iH commute,

$$U^\dagger U = e^{-iH}e^{iH} = e^{-iH+iH} = e^0 = I, \tag{2.55}$$

and similarly $UU^\dagger = I$. (However, in general, if $AB \neq BA$, then $e^A e^B \neq e^{A+B}$.)

If a unitary operator transforms two states

$$|\psi'\rangle = U|\psi\rangle, \tag{2.56a}$$
$$|\varphi'\rangle = U|\varphi\rangle, \tag{2.56b}$$

then their scalar product

$$\langle\psi'|\varphi'\rangle = \langle\psi|U^\dagger U|\varphi\rangle = \langle\psi|\varphi\rangle \tag{2.57}$$

is preserved.

2.3 Matrix Representations

If column matrices represent kets

$$|\psi\rangle \leftrightarrow \begin{bmatrix} a \\ b \end{bmatrix}, \tag{2.58}$$

then row matrices represent bras

$$\langle\psi| \leftrightarrow \begin{bmatrix} a^* & b^* \end{bmatrix} \leftrightarrow |\psi\rangle^\dagger, \tag{2.59}$$

square matrices represent ket bras

$$|\psi\rangle\langle\psi| \leftrightarrow \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} a^* & b^* \end{bmatrix} = \begin{bmatrix} aa^* & ab^* \\ ba^* & bb^* \end{bmatrix}, \tag{2.60}$$

and complex numbers or 1×1 matrices represent bra kets

$$\langle\psi|\psi\rangle = a^*a + b^*b \leftrightarrow \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a^*a + b^*b \end{bmatrix}, \tag{2.61}$$

where the color guides the eye in checking the matrix multiplication.

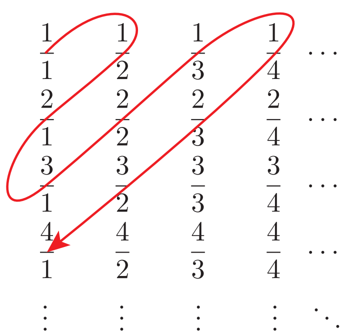
Table 2.1 summarizes the matrix representations. Bras map kets to numbers like *functionals*, while operators map kets to kets. The adjoint operation simultaneously generalizes complex conjugation and matrix transposition; even the adjoint symbol † is a kind of compromise between the complex conjugation symbol $*$ and the matrix transposition symbol T.

Table 2.1: Matrix representations for bra and kets.

vector	ket	$\|\psi\rangle$	$\begin{bmatrix} a \\ b \end{bmatrix}$
functional	bra	$\langle\psi\|$	$\begin{bmatrix} a^* & b^* \end{bmatrix}$
operator	ket bra	$\|\psi\rangle\langle\psi\|$	$\begin{bmatrix} aa^* & ab^* \\ ba^* & bb^* \end{bmatrix}$
scalar	bra ket	$\langle\psi\|\psi\rangle$	$a^*a + b^*b$

2.4 Uncountable Hilbert Spaces

Georg Cantor discovered [8] that there are different *degrees* of infinity. In particular, while rational numbers can be counted by placing them in one-to-one correspondence with natural numbers, the real numbers cannot, as in Fig. 2.1.



$$
\begin{aligned}
n_1 &= 0.d_{11}d_{12}d_{13}d_{14}\cdots \\
n_2 &= 0.d_{21}d_{22}d_{23}d_{24}\cdots \\
n_3 &= 0.d_{31}d_{32}d_{33}d_{34}\cdots \\
n_4 &= 0.d_{41}d_{42}d_{43}d_{44}\cdots \\
&\vdots \\
\tilde{n} &= 0.\tilde{d}_{11}\tilde{d}_{22}\tilde{d}_{33}\tilde{d}_{44}\cdots
\end{aligned}
$$

Figure 2.1: Cantor's first diagonal argument (left) counts the rational numbers, while Cantor's second diagonal argument (right) with $\tilde{d}_{nn} \neq d_{nn}$ proves the real numbers uncountable.

In an uncountably infinite Hilbert space, base states are labeled by uncountable, continuous indices, like $x \in \mathcal{R}$ for position, instead of countable, discrete indices like $n \in \mathcal{N}$. Linear superpositions involve uncountable, continuous sums or integrals

$$|\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle = \int dx\, |x\rangle\psi[x], \tag{2.62}$$

where $\psi[\,]$ is a *wave function*. Generalized functions express orthogonality

$$\langle x|y\rangle = \delta[x-y], \tag{2.63}$$

where the *Dirac delta*

$$\delta[x] = \lim_{\epsilon \to 0} \delta_\epsilon[x], \tag{2.64}$$

is the limit of infinitely tall, infinitesimally thin functions that bound a unit area,

$$\delta_\epsilon[x] = \left\{ \begin{array}{ll} 1/\epsilon & : |x| < \epsilon/2 \\ 0 & : |x| > \epsilon/2 \end{array} \right\}. \tag{2.65}$$

The Dirac delta's resulting normalization

$$1 = \int_{-\infty}^{\infty} dx\, \delta[x - x_0] \tag{2.66}$$

implies the *sifting property*

$$\int_{-\infty}^{\infty} dx\, \delta[x - x_0]\psi[x] = \psi[x_0] \int_{-\infty}^{\infty} dx\, \delta[x - x_0] = \psi[x_0]. \tag{2.67}$$

For example, project Eq. 2.62 onto the state $|y\rangle$ to get

$$\langle y|\psi\rangle = \int dx\, \langle y|x\rangle \psi[x] = \int dx\, \delta[x - y]\psi[x] = \psi[y]. \tag{2.68}$$

Table 2.2 compares countable and uncountable bases.

Table 2.2: Comparison between discrete and continuous bases formulas.

property	discrete or countable	continuous or uncountable
orthogonality	$\langle m\|n\rangle = \delta_{mn}$	$\langle x\|y\rangle = \delta[x - y]$
sifting	$\psi_n = \sum_m \psi_m \delta_{mn}$	$\psi[y] = \int_{-\infty}^{\infty} dx\, \delta[x - y]\psi[x]$
closure	$\|\psi\rangle = \sum_m \|m\rangle\langle m\|\psi\rangle$	$\|\psi\rangle = \int dx\, \|x\rangle\langle x\|\psi\rangle$

2.5 Quantum Example

As an example of the quantum Hilbert space formalism, with suggestively chosen notation, consider the energy observable H such that

$$H|\epsilon\rangle = \epsilon|\epsilon\rangle. \tag{2.69}$$

Since the operator $H = H^\dagger$ is hermitian, its eigenvalues $\epsilon = \epsilon^* \in \mathcal{H}$ are real. Assume an initial state as a symmetric superposition of orthonormal eigenstates

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}|\epsilon_1\rangle + \frac{1}{\sqrt{2}}|\epsilon_2\rangle \equiv |s\rangle \tag{2.70}$$

normalized such that

$$\begin{aligned}\langle\psi_0|\psi_0\rangle &= \left(\frac{1}{\sqrt{2}}\langle\epsilon_1| + \frac{1}{\sqrt{2}}\langle\epsilon_2|\right)\left(\frac{1}{\sqrt{2}}|\epsilon_1\rangle + \frac{1}{\sqrt{2}}|\epsilon_2\rangle\right)\\ &= \frac{1}{2}\langle\epsilon_1|\epsilon_1\rangle + \frac{1}{2}\langle\epsilon_1|\epsilon_2\rangle + \frac{1}{2}\langle\epsilon_2|\epsilon_1\rangle + \frac{1}{2}\langle\epsilon_2|\epsilon_2\rangle\\ &= \frac{1}{2} + 0 + 0 + \frac{1}{2}\\ &= 1. \end{aligned} \tag{2.71}$$

Given a norm-preserving unitary time translation operator

$$U_t = e^{-itH/\hbar}, \tag{2.72}$$

with real parameter $t \in \mathcal{R}$ and dimensional constant $\hbar$, the state at a later time

$$\begin{aligned}|\psi_t\rangle = U_t|\psi_0\rangle = e^{-itH/\hbar}|\psi_0\rangle &= \frac{1}{\sqrt{2}}e^{-itH/\hbar}|\epsilon_1\rangle + \frac{1}{\sqrt{2}}e^{-itH/\hbar}|\epsilon_2\rangle\\ &= \frac{1}{\sqrt{2}}e^{-it\epsilon_1/\hbar}|\epsilon_1\rangle + \frac{1}{\sqrt{2}}e^{-it\epsilon_2/\hbar}|\epsilon_2\rangle. \end{aligned} \tag{2.73}$$

The amplitude for again observing the initial symmetric state is the projection

$$\begin{aligned}\langle s|\psi_t\rangle &= \left(\frac{1}{\sqrt{2}}\langle\epsilon_1| + \frac{1}{\sqrt{2}}\langle\epsilon_2|\right)\left(\frac{1}{\sqrt{2}}e^{-it\epsilon_1/\hbar}|\epsilon_1\rangle + \frac{1}{\sqrt{2}}e^{-it\epsilon_2/\hbar}|\epsilon_2\rangle\right)\\ &= \frac{1}{2}e^{-it\epsilon_1/\hbar} + \frac{1}{2}e^{-it\epsilon_2/\hbar}, \end{aligned} \tag{2.74}$$

and the probability is the absolute square

$$\begin{aligned}\mathcal{P}_s &= |\langle s|\psi_t\rangle|^2\\ &= \left(\frac{1}{2}e^{+it\epsilon_1/\hbar} + \frac{1}{2}e^{+it\epsilon_2/\hbar}\right)\left(\frac{1}{2}e^{-it\epsilon_1/\hbar} + \frac{1}{2}e^{-it\epsilon_2/\hbar}\right)\\ &= \frac{1}{4} + \frac{1}{4}e^{+it(\epsilon_1-\epsilon_2)/\hbar} + \frac{1}{4}e^{-it(\epsilon_1-\epsilon_2)/\hbar} + \frac{1}{4}\\ &= \frac{1}{2} + \frac{1}{2}\cos\left[t\frac{\epsilon_1-\epsilon_2}{\hbar}\right]\\ &= \cos^2\left[\frac{\epsilon_1-\epsilon_2}{2\hbar}t\right]. \end{aligned} \tag{2.75}$$

In quantum mechanics, normalized vectors represent states and complex vector projections represent probability amplitudes. The absolute square of amplitudes represent probabilities. Hermitian operators represent observables and their real eigenvalues represent observed values. Unitary operators represent transformations like translations and rotations.

2.6 Commutation

Let $A = A^\dagger$ and $B = B^\dagger$ be Hermitian operators representing observable quantities like energy and momentum. If they commute, so that $AB = BA$ and their *commutator*

$$[A, B] = AB - BA = 0 \tag{2.76}$$

vanishes, then they share common eigenstates and can be known exactly simultaneously. If they do not commute, the measurement of one "contaminates" measurement of the other, and perfectly knowing one leaves the other completely indeterminate.

Assume the operators do commute, and let $|a\rangle$ be an eigenstate of A with eigenvalue a,

$$A|a\rangle = a|a\rangle. \tag{2.77}$$

The vanishing of the commutator implies the vanishing of the matrix elements

$$0 = \langle a|[A, B]|a'\rangle = \langle a|AB|a'\rangle - \langle a|BA|a'\rangle = (a - a')\langle a|B|a'\rangle. \tag{2.78}$$

If the eigenvalues $a \neq a'$ are nondegenerate (or can be made so), then $\langle a|B|a'\rangle = 0$ and the operator B is "diagonal" in the $\{|a\rangle\}$ basis,

$$\langle a|B|a'\rangle = B_{aa'}\delta_{aa'} \equiv b\langle a|a'\rangle. \tag{2.79}$$

Since this is true for all $|a\rangle$,

$$B|a'\rangle = b|a'\rangle, \tag{2.80}$$

and $|a'\rangle = |a', b\rangle$ is also an eigenstate of B,

$$A|a, b\rangle = a|a, b\rangle, \tag{2.81a}$$
$$B|a, b\rangle = b|a, b\rangle. \tag{2.81b}$$

Now assume the operators do *not* commute. If the state $|\psi\rangle = \sum |a\rangle\psi_a \in \mathcal{H}$ characterizes the system, then the probability of measuring the observable corresponding to the operator A and getting the result a is

$$\mathcal{P}_a = |\langle a|\psi\rangle|^2 = |\psi_a|^2, \tag{2.82}$$

the average or mean of many such measurements on identical systems is

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \sum_{a,a'}\langle a'|A|a\rangle\psi^*_{a'}\psi_a = \sum_{a,a'} a\delta_{a',a}\psi^*_{a'}\psi_a = \sum_a a|\psi_a|^2 = \sum_a a\mathcal{P}_a, \tag{2.83}$$

and the spread or uncertainty in the results is the standard deviation

$$\Delta A = \sqrt{\langle(A - \langle A\rangle I)^2\rangle} = \sqrt{\langle(A - \langle A\rangle)^2\rangle}. \tag{2.84}$$

Remove the mean from the operators by defining

$$A_0 = A - \langle A\rangle, \tag{2.85a}$$
$$B_0 = B - \langle B\rangle. \tag{2.85b}$$

Define the linear combination

$$C_0 = A_0 - i\epsilon B_0, \tag{2.86}$$

where $\epsilon \in \mathcal{R}$ is a real number, and the state

$$|\varphi\rangle = C_0|\psi\rangle \tag{2.87}$$

so that

$$\begin{aligned} 0 \leq \langle\varphi|\varphi\rangle &= \langle\psi|C_0^\dagger C_0|\psi\rangle \\ &= \langle\psi|(A_0 + i\epsilon B_0)(A_0 - i\epsilon B_0)|\psi\rangle \\ &= \langle\psi|A_0^2 - i\epsilon A_0 B_0 + i\epsilon B_0 A_0 + \epsilon^2 B_0^2|\psi\rangle \\ &= \langle A_0^2\rangle - \epsilon\langle i[A_0, B_0]\rangle + \epsilon^2\langle B_0^2\rangle \\ &= \mathit{\Delta} A^2 - \epsilon\langle i[A, B]\rangle + \epsilon^2 \mathit{\Delta} B^2. \end{aligned} \tag{2.88}$$

This quadratic equation in ϵ defines a vertical parabola confined to the upper-half plane. Since it cannot cross the ϵ axis, it cannot have two real roots, and its quadratic discriminant must be non-positive,

$$D = \langle i[A, B]\rangle^2 - 4\mathit{\Delta} A^2 \mathit{\Delta} B^2 \leq 0. \tag{2.89}$$

Hence, the product of the uncertainties

$$\mathit{\Delta} A\, \mathit{\Delta} B \geq \frac{1}{2}\left|\big\langle i[A, B]\big\rangle\right|, \tag{2.90}$$

which is conventionally known as the (generalized) *Heisenberg uncertainty principle.* For example, if two operators Q and P have the commutator

$$[Q, P] = i\hbar I, \tag{2.91}$$

then the products of the uncertainties in measurements of the corresponding observables satisfy

$$\mathit{\Delta} Q\, \mathit{\Delta} P \geq \frac{1}{2}\hbar, \tag{2.92}$$

so if one is certain, say $\mathit{\Delta} Q = 0$, the other is indeterminate, $\mathit{\Delta} P = \infty$.

Problems

1. Given the states

$$|\psi\rangle = 3i|1\rangle + 2|2\rangle, \tag{2.93a}$$
$$|\varphi\rangle = 2|1\rangle + i|2\rangle, \tag{2.93b}$$

and the Section 2.3 standard matrix representation

$$\langle 1| \leftrightarrow \boxed{\begin{array}{cc} 1 & 0 \end{array}}, \tag{2.94a}$$
$$\langle 2| \leftrightarrow \boxed{\begin{array}{cc} 0 & 1 \end{array}}, \tag{2.94b}$$

evaluate the following both with *and* without the representation.

(a) $\langle\psi|\varphi\rangle$

(b) $\langle\varphi|\psi\rangle$

(c) $|\psi\rangle\langle\varphi|$

(d) $|\varphi\rangle\langle\psi|$

2. Given the operator and states

$$A = i|1\rangle\langle 1| + |1\rangle\langle 2| + 2|2\rangle\langle 1| + 3|2\rangle\langle 2|, \tag{2.95a}$$
$$|\psi\rangle = |1\rangle + i|2\rangle \tag{2.95b}$$
$$|\varphi\rangle = 2|1\rangle + |2\rangle, \tag{2.95c}$$

verify that $\langle\psi|A^\dagger|\varphi\rangle = \langle\varphi|A|\psi\rangle^*$ both with *and* without a matrix representation.

3. Simplify the following by removing the dagger †. Assume $c \in \mathcal{C}$ is a complex number and all the operators are hermitian, as in Section 2.2.4.

(a) $c^\dagger$

(b) $(A|\psi\rangle)^\dagger$

(c) $\langle\psi|A|\varphi\rangle^\dagger$

(d) $(c\langle\phi|A|\psi\rangle|\chi\rangle\langle\psi|)^\dagger$

(e) $(|\psi\rangle = \sum_n |n\rangle\psi_n)^\dagger$

(f) $\left(|\varphi\rangle = \int dx\, |x\rangle\varphi[x]\right)^\dagger$

(g) $\left(A^\dagger B^\dagger C^\dagger\right)^\dagger$

4. Simplify the following by removing the deltas.

(a) $\sum_{n=1}^{\infty} n^2 \delta_{mn}$

(b) $\int_{-\infty}^{\infty} dx\, x^2 \delta[x-y]$

(c) $\int_{-\infty}^{\infty} dx\, e^{ikx}\delta[x]$

(d) $\sum_{n=1}^{N} \delta_{mn}$ (Hint: 2 cases.)

(e) $\int_{-\infty}^{z} dx\, \delta[x-y]$ (Hint: 2 cases.)

5. Let $P_n = |n\rangle\langle n|$ be a projection operator onto a 2-dimensional Hilbert space.

   (a) Prove that $P_n^2 = P_n$, and interpret this result graphically.

   (b) Prove that P_n is hermitian.

   (c) What are the (real!) eigenvalues of P_n?

   (d) Find a matrix representation for P_n.

   (e) Find a matrix representation for $\sum_n P_n = \sum_n |n\rangle\langle n|$. Surprised?

6. Let $\sigma_y = -i|1\rangle\langle 2| + i|2\rangle\langle 1|$ be a Pauli operator.

   (a) Prove that σ_y is hermitian.

   (b) Find its eigenstates and eigenvalues.

   (c) Verify that its eigenvalues are real and its eigenstates are orthogonal.

   (d) Find projection operators P_n onto the *normalized* eigenstates.

   (e) Verify that these projectors satisfy the closure relation $P_1 + P_2 = I$.

7. Let $\sigma_x = |1\rangle\langle 2| + |2\rangle\langle 1|$ be another Pauli operator.

   (a) Prove that $H = \alpha\sigma_x$ is hermitian, where $\alpha \in \mathcal{R}$ is a real parameter.

   (b) Prove that $U = I\cos\alpha + i\sigma_x \sin\alpha$ is unitary.

   (c) Verify that $U = e^{iH}$ or equivalently $I\cos\alpha + i\sigma_x\sin\alpha = e^{i\alpha\sigma_x}$.

8. Repeat the Section 2.5 quantum example with the antisymmetric initial state

$$|a\rangle = \frac{1}{\sqrt{2}}|\epsilon_1\rangle - \frac{1}{\sqrt{2}}|\epsilon_2\rangle. \tag{2.96}$$

9. Show that if two operators share common eigenstates, as in Eq. 2.81, they commute.

Chapter 3

Symmetry Commutators

Fundamental physical variables like energy and momentum are intimately related to spacetime symmetry transformations [11, 12].

3.1 Spacetime Symmetries

Something is symmetric if it is invariant under a transformation. For example, a sphere is unchanged by rotations about its center. Nonrelativistic physics is invariant under the *Galilei group* of spacetime transformations, which consists of translations, rotations, and boosts. If the column matrix

$$\vec{x}_t \leftrightarrow \begin{bmatrix} x_0 \\ \hline x_1 \\ x_2 \\ x_3 \\ \hline 1 \end{bmatrix} = \begin{bmatrix} t \\ \hline x \\ y \\ z \\ \hline 1 \end{bmatrix} \leftrightarrow \vec{r}_t \tag{3.1}$$

represents an event in spacetime, then a space translation through a distance δ in the y-direction is

$$S_{\hat{y}\delta} \begin{bmatrix} t \\ \hline x \\ y \\ z \\ \hline 1 \end{bmatrix} = \left[\begin{array}{c|ccc|c} 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & \delta \\ 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \end{array}\right] \begin{bmatrix} t \\ \hline x \\ y \\ z \\ \hline 1 \end{bmatrix} = \begin{bmatrix} t \\ \hline x \\ y+\delta \\ z \\ \hline 1 \end{bmatrix}, \tag{3.2}$$

where the color guides the eye in checking the matrix multiplication. A time translation through a duration ϵ is

$$T_\epsilon \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|ccc|c|}\hline 1 & 0 & 0 & 0 & \epsilon \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \\ \hline\end{array} \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|}\hline t+\epsilon \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array}, \tag{3.3}$$

A space rotation through an angle θ about the x-direction is

$$R_{\hat{x}\theta} \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|ccc|c|}\hline 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \cos\theta & -\sin\theta & 0 \\ 0 & 0 & \sin\theta & \cos\theta & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \\ \hline\end{array} \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|}\hline t \\ \hline x \\ y\cos\theta - z\sin\theta \\ y\sin\theta + z\cos\theta \\ \hline 1 \\ \hline\end{array}. \tag{3.4}$$

The orthogonal rotations are cyclic permutations of the rows and columns of the 3×3 space part of the rotation matrix, as in Problem 3.1. A boost by a speed v in the y-direction is

$$B_{\hat{y}v} \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|ccc|c|}\hline 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 \\ v & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 1 \\ \hline\end{array} \begin{array}{|c|}\hline t \\ \hline x \\ y \\ z \\ \hline 1 \\ \hline\end{array} = \begin{array}{|c|}\hline t \\ \hline x \\ y+vt \\ z \\ \hline 1 \\ \hline\end{array}. \tag{3.5}$$

Boosts or velocity translations connect references frames in relative motion. Figure 3.1 compares Galilei boosts with space rotations and spacetime rotations, which are the Lorentz transformations of special relativity, as well as with space translations.

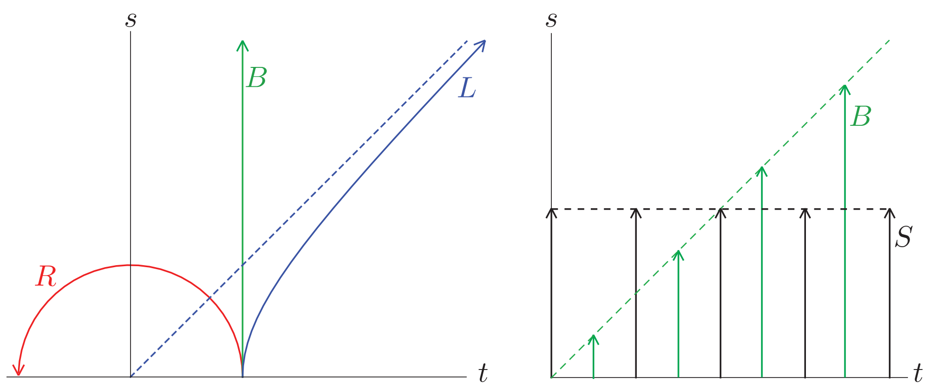


Figure 3.1: Active Galilei boost B compared with a Lorentz boost L and a rotation R (left) and translations S (right) in 1+1 dimensional spacetime $\{t, s\}$.

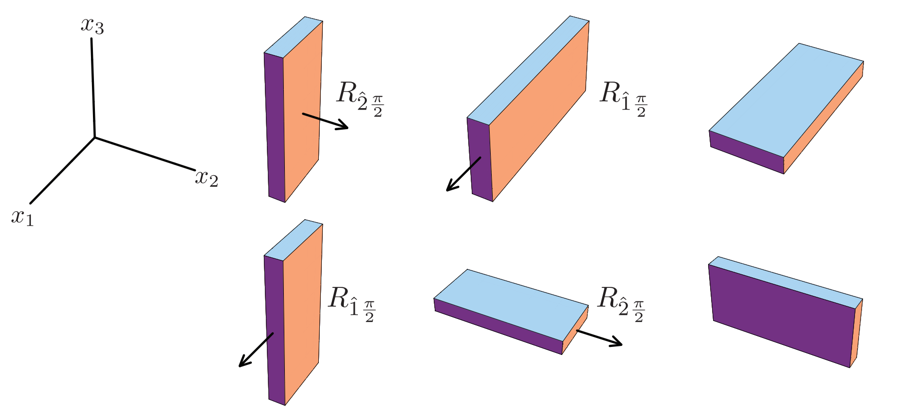


Figure 3.2: Finite rotations about different axes do not commute, as the final orientation depends on the order of the rotations.

3.2 Spacetime Closures

Abbreviate $S[\hat{x}_a \epsilon] = S_{\hat{x}_a \epsilon} = S_{\hat{a}\epsilon} = S_a$, and so on. The 10 spacetime transformations

$$\mathcal{T}_a \in \{T, S_1, S_2, S_3, R_1, R_2, R_3, B_1, B_2, B_3\} \tag{3.6}$$

form a group because inverses $\mathcal{T}_a^{-1}$ and an identity I exist, and because any two successive transformations is equivalent to a third, $\mathcal{T}_c = \mathcal{T}_b \mathcal{T}_a$. However, some of the spacetime transformations do not commute,

$$\mathcal{T}_b \mathcal{T}_a \neq \mathcal{T}_a \mathcal{T}_b \tag{3.7}$$

or

$$\mathcal{T}_b \mathcal{T}_a - \mathcal{T}_a \mathcal{T}_b = [\mathcal{T}_a, \mathcal{T}_b] \neq 0. \tag{3.8}$$

or

$$\mathcal{T}_b^{-1}\mathcal{T}_a^{-1}\mathcal{T}_b\mathcal{T}_a \neq I. \tag{3.9}$$

For example, rotating a book 90° about its cover and then 90° about its spine orients it differently than rotating it 90° about its spine and then 90° about its cover, as in Fig. 3.2.

For small translations, rotations, and boosts, by amounts $\epsilon \ll 1$, Fig 3.3 illustrates the nontrivial commutators. To $\mathcal{O}[\epsilon^2]$, $\sin\epsilon = \epsilon$ and $\cos\epsilon = 1 - \frac{1}{2}\epsilon^2$. Hence, for successive rotations about orthogonal axes,

$$
\begin{aligned}
&R_{\hat{2}\epsilon}^{-1}R_{\hat{3}\epsilon}^{-1}R_{\hat{2}\epsilon}R_{\hat{3}\epsilon} \\
&= R_{\hat{2}\epsilon}^{-1}R_{\hat{3}\epsilon}^{-1}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & 0 & \epsilon & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & -\epsilon & 0 & 1-\frac{1}{2}\epsilon^2 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & -\epsilon & 0 & 0 \\
0 & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= R_{\hat{2}\epsilon}^{-1}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & \epsilon & 0 & 0 \\
0 & -\epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\epsilon^2 & -\epsilon & \epsilon & 0 \\
0 & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & -\epsilon & \epsilon^2 & 1-\frac{1}{2}\epsilon^2 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & 0 & -\epsilon & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & \epsilon & 0 & 1-\frac{1}{2}\epsilon^2 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & 0 & \epsilon & 0 \\
0 & 0 & 1 & -\epsilon^2 & 0 \\
0 & -\epsilon & \epsilon^2 & 1-\frac{1}{2}\epsilon^2 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & -\epsilon^2 & 0 \\
0 & 0 & \epsilon^2 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= R_{\hat{1}\epsilon^2},
\end{aligned} \tag{3.10}
$$

where the colors help guide the eye in checking the matrix multiplication. Geometrically, this gap arises because the rotations and their inverses involve circles of different radii, as in Fig. 3.3. It can be closed by a single orthogonal rotation. (Space rotations are a subgroup of the Galilei group.)

For a rotation followed by a translation,

$$
\begin{aligned}
&S^{-1}_{\hat{2}\epsilon} R^{-1}_{\hat{3}\epsilon} S_{\hat{2}\epsilon} R_{\hat{3}\epsilon} \\
&= S^{-1}_{\hat{2}\epsilon} R^{-1}_{\hat{3}\epsilon}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & \epsilon \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & -\epsilon & 0 & 0 \\
0 & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= S^{-1}_{\hat{2}\epsilon}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & \epsilon & 0 & 0 \\
0 & -\epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & -\epsilon & 0 & 0 \\
0 & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & \epsilon \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & -\epsilon \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & \epsilon^2 \\
0 & 0 & 1 & 0 & \epsilon \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & \epsilon^2 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= S_{\hat{1}\epsilon^2}. \qquad (3.11)
\end{aligned}
$$

Geometrically, this gap arises because the rotation and its inverse involve circles of different radii, as in Fig. 3.3. It can be closed by a single translation.

For a rotation followed by a boost,

$$
\begin{aligned}
& B^{-1}_{\hat{2}\epsilon} R^{-1}_{\hat{3}\epsilon} B_{\hat{2}\epsilon} R_{\hat{3}\epsilon} \\
&= B^{-1}_{\hat{2}\epsilon} R^{-1}_{\hat{3}\epsilon}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
\epsilon & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & -\epsilon & 0 & 0 \\
0 & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= B^{-1}_{\hat{2}\epsilon}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & \epsilon & 0 & 0 \\
0 & -\epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1-\frac{1}{2}\epsilon^2 & -\epsilon & 0 & 0 \\
\epsilon & \epsilon & 1-\frac{1}{2}\epsilon^2 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
-\epsilon & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
\epsilon^2 & 1 & 0 & 0 & 0 \\
\epsilon & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
\epsilon^2 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= B_{\hat{1}\epsilon^2}.
\end{aligned} \tag{3.12}
$$

Geometrically, this gap arises again because the rotation and its inverse involve circles of different radii, as in Fig. 3.3. It can be closed by a single boost.

For a time translation followed by a boost,

$$
\begin{aligned}
&B_{\hat{2}\epsilon}^{-1} T_{\epsilon}^{-1} B_{\hat{2}\epsilon} T_{\epsilon} \\
&= B_{\hat{2}\epsilon}^{-1} T_{\epsilon}^{-1}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
\epsilon & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & \epsilon \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= B_{\hat{2}\epsilon}^{-1}
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & -\epsilon \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & \epsilon \\ \hline
0 & 1 & 0 & 0 & 0 \\
\epsilon & 0 & 1 & 0 & \epsilon^2 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
-\epsilon & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right]
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
\epsilon & 0 & 1 & 0 & \epsilon^2 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&=
\left[\begin{array}{c|ccc|c}
1 & 0 & 0 & 0 & 0 \\ \hline
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & \epsilon^2 \\
0 & 0 & 0 & 1 & 0 \\ \hline
0 & 0 & 0 & 0 & 1
\end{array}\right] \\
&= S_{\hat{2}\epsilon^2}.
\end{aligned}
\tag{3.13}
$$

Geometrically, this gap arises because the boost and its inverse involve different times, as in Fig. 3.3. It can be closed by a single space translation.

All other spacetime transformations commute, as is summarized in Table 3.1, where the *Levi-Civita symbol* $\epsilon_{123} = 1$ is antisymmetric on interchange of any index (so it vanishes if any two indices are the same) and repeated indices are summed over.

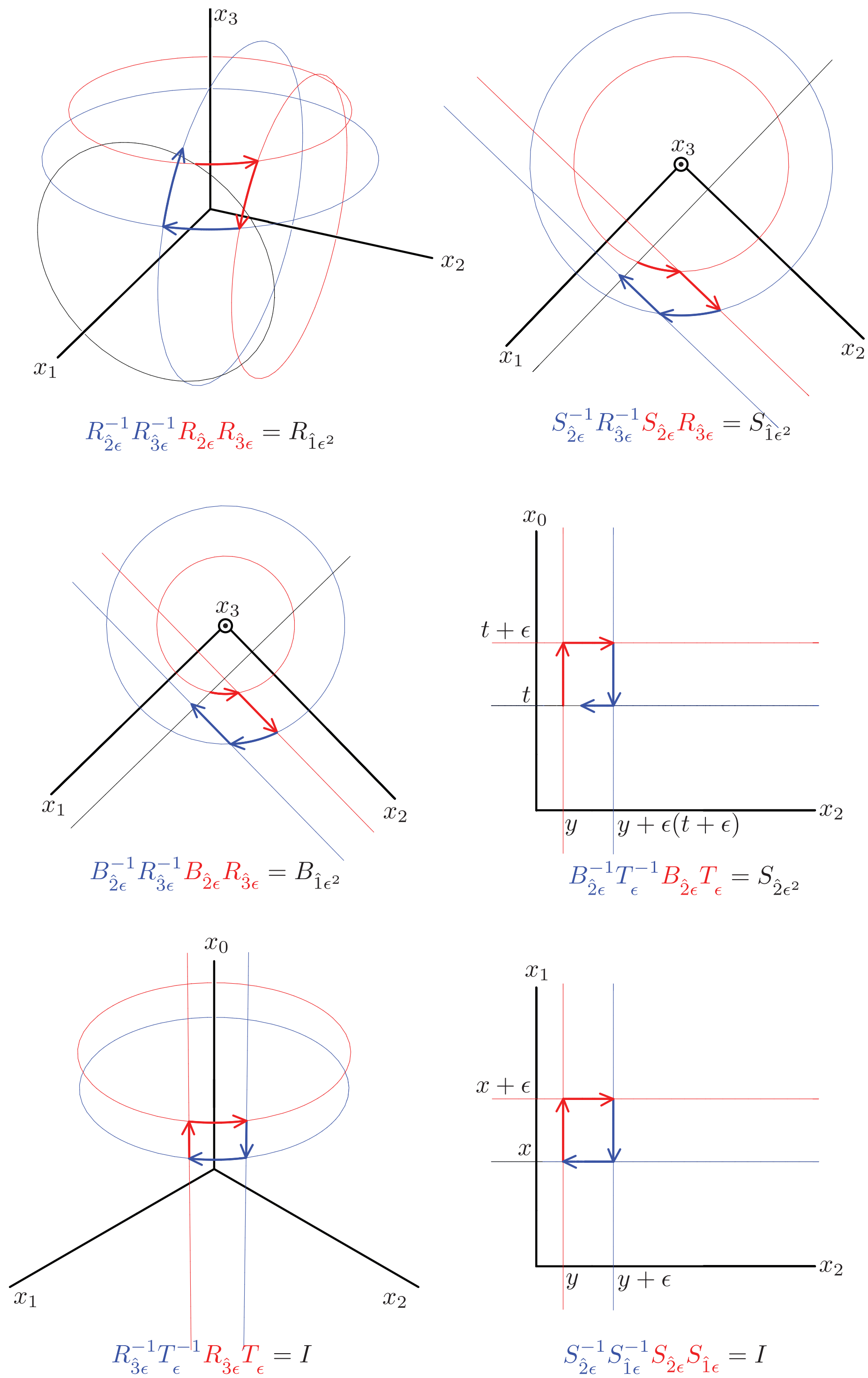


Figure 3.3: Some spacetime transformations do not commute (top four examples), while others do (bottom two examples).

Table 3.1: Summary of nontrivial spacetime closures to $\mathcal{O}[\epsilon^2]$.

$S_a^{-1}S_b^{-1}S_aS_b = I$	$R_a^{-1}T^{-1}R_aT = I$	$R_a^{-1}R_b^{-1}R_aR_b = \epsilon_{abc}R_c$
$B_a^{-1}B_b^{-1}B_aB_b = I$	$S_a^{-1}T^{-1}S_aT = I$	$R_a^{-1}S_b^{-1}R_aS_b = \epsilon_{abc}S_c$
$B_a^{-1}S_b^{-1}B_aS_b = I$	$B_a^{-1}T^{-1}B_aT = S_a$	$R_a^{-1}B_b^{-1}R_aB_b = \epsilon_{abc}B_c$

3.3 State Space Symmetry Generators

3.3.1 Generic Commutator

Every spacetime transformation

$$\mathcal{T}\vec{r}_t = \vec{r}_t{}', \tag{3.14}$$

corresponds a state space unitary transformation

$$U[\mathcal{T}]\,|\psi\rangle = |\psi'\rangle\,. \tag{3.15}$$

A hermitian operator $H = H^\dagger$ generates each unitary transformation $U^{-1} = U^\dagger$ of size ϵ by

$$U\left[\mathcal{T}_\epsilon\right] = e^{i\epsilon H} = I + i\epsilon H - \frac{1}{2}\epsilon^2 H^2 + \cdots\,, \tag{3.16}$$

where

$$\left.\frac{dU}{d\epsilon}\right|_{\epsilon=0} = iH \equiv i\mathcal{T}'_\epsilon. \tag{3.17}$$

Successive spacetime transformations and their inverses

$$\mathcal{T}_{\hat{b}\epsilon}^{-1}\mathcal{T}_{\hat{a}\epsilon}^{-1}\mathcal{T}_{\hat{b}\epsilon}\mathcal{T}_{\hat{a}\epsilon} = \mathcal{T}_{\hat{c}\epsilon^2} \tag{3.18}$$

correspond on state space to

$$U\left[\mathcal{T}_{\hat{b}\epsilon}^{-1}\right]U\left[\mathcal{T}_{\hat{a}\epsilon}^{-1}\right]U\left[\mathcal{T}_{\hat{b}\epsilon}\right]U\left[\mathcal{T}_{\hat{a}\epsilon}\right] = U\left[\mathcal{T}_{\hat{c}\epsilon^2}\right], \tag{3.19}$$

In terms of the generators,

$$e^{-i\epsilon H_b}e^{-i\epsilon H_a}e^{i\epsilon H_b}e^{i\epsilon H_a} = e^{i\epsilon^2 H_c}, \tag{3.20}$$

which to $\mathcal{O}[\epsilon^2]$ is

$$
\begin{aligned}
&I + i\epsilon^2 H_c \\
&= \left(I - i\epsilon H_b - \frac{1}{2}\epsilon^2 H_b^2\right)\left(I - i\epsilon H_a - \frac{1}{2}\epsilon^2 H_a^2\right) \times \\
&\quad \left(I + i\epsilon H_b - \frac{1}{2}\epsilon^2 H_b^2\right)\left(I + i\epsilon H_a - \frac{1}{2}\epsilon^2 H_a^2\right) \\
&= \left(I - i\epsilon(H_b + H_a) - \epsilon^2 H_b H_a - \frac{1}{2}\epsilon^2 (H_b^2 + H_a^2)\right) \times \\
&\quad \left(I + i\epsilon(H_b + H_a) - \epsilon^2 H_b H_a - \frac{1}{2}\epsilon^2 (H_b^2 + H_a^2)\right) \\
&= I - 2\epsilon^2 H_b H_a + \epsilon^2(\cancel{H_b^2} + H_b H_a + H_a H_b + \cancel{H_a^2}) - \epsilon^2(\cancel{H_b^2} + \cancel{H_a^2}) \\
&= I + \epsilon^2(-H_b H_a + H_a H_b) \\
&= I + \epsilon^2 [H_a, H_b],
\end{aligned}
\tag{3.21}
$$

so the commutator of the hermitian generators

$$[H_a, H_b] = iH_c. \tag{3.22}$$

However, a shift of $H_a \to H_a + \varphi I$ in the generators implies an unobservable shift $|\varphi\rangle \to e^{i\varphi}|\psi\rangle$ in the states along with the more general commutator

$$[H_a, H_b] = iH_c + i\varphi I. \tag{3.23}$$

3.3.2 Commutator Antisymmetries

Commutators, and commutators involving commutators, are antisymmetric. Add

$$[A, B] = \cancel{AB} - \cancel{BA}, \tag{3.24a}$$
$$[B, A] = \cancel{BA} - \cancel{AB}, \tag{3.24b}$$

to get

$$[A, B] + [B, A] = 0 \tag{3.25}$$

or

$$[A, B] = -[B, A]. \tag{3.26}$$

Add

$$[[A, B], C] = [AB - BA, C] = \cancel{ABC} - \cancel{BAC} - \cancel{CAB} + \cancel{CBA}, \tag{3.27a}$$
$$[[C, A], B] = [CA - AC, B] = \cancel{CAB} - \cancel{ACB} - \cancel{BCA} + \cancel{BAC}, \tag{3.27b}$$
$$[[B, C], A] = [BC - CB, A] = \cancel{BCA} - \cancel{CBA} - \cancel{ABC} + \cancel{ACB}, \tag{3.27c}$$

to get the *Jacobi identity*

$$[[A,B],C]+[[B,C],A]+[[C,A],B]=0 \tag{3.28}$$

or

$$[[A,B],C]=[[C,B],A]+[[A,C],B]. \tag{3.29}$$

Furthermore, commutators of hermitian operators are antihermitian. Assume $A^\dagger = A$ and $B^\dagger = B$. If $[A,B]=C$, then

$$C^\dagger = (AB-BA)^\dagger = (AB)^\dagger-(BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA-AB=-C. \tag{3.30}$$

Thus, if $[A,B]=iH$, then H is hermitian.

3.3.3 Phase Constants

Table 3.2 summarizes the tentative generator commutation relations with the real phase constants $\varphi^n_{ab} \in \mathcal{R}$ (where n is an index and not an exponent). The commutator relations allow the phase constants to be zeroed in all but one case.

Table 3.2: Nontrivial symmetry generator commutators with phase constants.

$[S'_a,S'_b]=i\varphi^1_{ab}I$	$[R'_a,T']=i\varphi^4_{a0}I$	$[R'_a,R'_b]=i\epsilon_{abc}R'_c+i\varphi^7_{ab}I$
$[B'_a,B'_b]=i\varphi^2_{ab}I$	$[S'_a,T']=i\varphi^5_{a0}I$	$[R'_a,S'_b]=i\epsilon_{abc}S'_c+i\varphi^8_{ab}I$
$[B'_a,S'_b]=i\varphi^3_{ab}I$	$[B'_a,T']=iS'_a+i\varphi^6_{a0}I$	$[R'_a,B'_b]=i\epsilon_{abc}B'_c+i\varphi^9_{ab}I$

Eliminable

Commutator antisymmetry implies that every operator commutes with itself, $[A,A]=-[A,A]$ implies $[A,A]=0$. Hence $\varphi^n_{aa}=0$.

In fact, all the phase constants in the red top left corner of Table 3.2 can be eliminated by antisymmetry. Since the constants commute with everything, the Eq. 3.28 Jacobi antisymmetry of $\{R'_2,S'_3,T'\}$,

$$\begin{aligned} 0 &= [[R'_2,S'_3],T']+[[T',R'_2],S'_3]+[[S'_3,T'],R'_2], \\ &= i[S'_1,T']-i\varphi^4_{20}[I,S'_3]+i\varphi^5_{30}[I,R'_2], \\ &= -\varphi^5_{10}I-0+0, \end{aligned} \tag{3.31}$$

implies

$$0=[S'_a,T']=i\varphi^5_{a0}I. \tag{3.32}$$

Similarly,

$$0=[R'_a,T']=i\varphi^4_{a0}I, \tag{3.33}$$

$$0=[S'_a,S'_b]=i\varphi^1_{ab}I, \tag{3.34}$$

$$0=[B'_a,B'_b]=i\varphi^2_{ab}I. \tag{3.35}$$

Absorbable

The phase constants in the blue last column of Table 3.2 can be absorbed into the symmetry generators. Antisymmetry of the rotation-rotation commutator

$$i\epsilon_{bac}R'_c + i\varphi^7_{ba}I = -i\epsilon_{abc}R'_c - i\varphi^7_{ab}I \tag{3.36}$$

implies the antisymmetry of the corresponding phase constant

$$\varphi^7_{ba} = -\varphi^7_{ab} \equiv \epsilon_{abc}\varphi^7_c. \tag{3.37}$$

Then the substitution

$$R'_a \to R'_a - \varphi^7_a I, \tag{3.38}$$

which is equivalent to the unobservable global phase change

$$|\psi'\rangle = e^{-i\varphi^7_a}|\psi\rangle, \tag{3.39}$$

converts the commutator

$$[R'_a, R'_b] = i\epsilon_{abc}R'_c + i\epsilon_{abc}\varphi^7_c I \tag{3.40}$$

into

$$[R'_a, R'_b] = i\epsilon_{abc}R'_c. \tag{3.41}$$

Next, the Jacobi antisymmetry of $\{R'_1, R'_2, B'_3\}$,

$$\begin{aligned} 0 &= [[R'_1, R'_2], B'_3] + [[B'_3, R'_1], R'_2] + [[R'_2, B'_3], R'_1], \\ &= i[R'_3, B'_3] - i[B'_2, R'_2] + i[B'_1, R'_1], \end{aligned} \tag{3.42}$$

implies, by cyclically permuting the space axes,

$$0 = +[R'_3, B'_3] - [B'_2, R'_2] + [B'_1, R'_1], \tag{3.43a}$$

$$0 = +[R'_1, B'_1] - [B'_3, R'_3] + [B'_2, R'_2]. \tag{3.43b}$$

Adding implies $[R'_3, B'_3] = 0$ and similarly

$$[R'_a, B'_a] = 0. \tag{3.44}$$

Using this result, the Jacobi antisymmetry of $\{R'_3, R'_1, B'_3\}$,

$$\begin{aligned} 0 &= [[R'_3, R'_1], B'_3] + [[B'_3, R'_3], R'_1] + [[R'_1, B'_3], R'_3], \\ &= i[R'_2, B'_3] + i[0, R'_1] - i[B'_2, R'_3], \end{aligned} \tag{3.45}$$

implies the index antisymmetry of the commutator

$$[R'_a, B'_b] = -[R'_b, B'_a] \tag{3.46}$$

and the antisymmetry of the corresponding phase constant

$$\varphi^9_{ba} = -\varphi^9_{ab} \equiv \epsilon_{abc}\varphi^9_c. \tag{3.47}$$

Then the substitution

$$B'_a \to B'_a - \varphi^9_a I \tag{3.48}$$

converts the commutator

$$[R'_a, B'_b] = i\epsilon_{abc} B'_c + i\epsilon_{abc}\varphi^9_c I \tag{3.49}$$

into

$$[R'_a, B'_b] = i\epsilon_{abc} B'_c. \tag{3.50}$$

A similar procedure yields

$$[R'_a, S'_b] = i\epsilon_{abc} S'_c. \tag{3.51}$$

These results imply that phase constant in the teal middle bottom of Table 3.2 can be eliminated. The Jacobi antisymmetry of $\{R'_1, B'_2, T'\}$,

$$\begin{aligned} 0 &= [[R'_1, B'_2], T'] + [[T', R'_1], B'_2] + [[B'_2, T'], R'_1] \\ &= i[B'_3, T'] + [0, B'_2] + i[S'_2, R'_1] \\ &= i[B'_3, T'] + 0 + S'_3, \end{aligned} \tag{3.52}$$

implies, by cycling axes,

$$[B'_a, T'] = iS'_a. \tag{3.53}$$

Irremovable

The final unaccounted phase constant is in the black bottom left corner of Table 3.2. The Jacobi antisymmetry of $\{R'_1, B'_2, S'_1\}$,

$$\begin{aligned} 0 &= [[R'_1, B'_2], S'_1] + [[S'_1, R'_1], B'_2] + [[B'_2, S'_1], R'_1] \\ &= i[B'_3, S'_1] + [0, B'_2] + i\varphi^3_{21}[I, R'_1] \\ &= i[B'_3, S'_1] + 0 + 0, \end{aligned} \tag{3.54}$$

implies, by cycling axes,

$$[B'_a, S'_b] = 0, \tag{3.55}$$

for $a \neq b$. The Jacobi antisymmetry of $\{R'_1, B'_2, S'_3\}$,

$$\begin{aligned} 0 &= [[R'_1, B'_2], S'_3] + [[S'_3, R'_1], B'_2] + [[B'_2, S'_3], R'_1] \\ &= i[B'_3, S'_3] + i[S'_2, B'_2] + i\varphi^3_{23}[I, R'_1] \\ &= i[B'_3, S'_3] + i[S'_2, B'_2] + 0, \end{aligned} \tag{3.56}$$

implies, by cycling axes,

$$[B'_a, S'_a] = [B'_b, S'_b]. \tag{3.57}$$

Combine Eq. 3.55 and Eq. 3.57 to write

$$[B'_a, S'_b] = i\delta_{ab}\mu I, \tag{3.58}$$

where μ is a real but undetermined constant, and the *Kronecker symbol* δ_{ab} is unity if its indices are the same but is zero otherwise. Table 3.3 summarizes the final generator commutation relations.

Table 3.3: Nontrivial symmetry generator commutators.

$[S'_a, S'_b] = 0$	$[R'_a, T'] = 0$	$[R'_a, R'_b] = i\epsilon_{abc}R'_c$
$[B'_a, B'_b] = 0$	$[S'_a, T'] = 0$	$[R'_a, S'_b] = i\epsilon_{abc}S'_c$
$[B'_a, S'_b] = i\delta_{ab}\mu I$	$[B'_a, T'] = iS'_a$	$[R'_a, B'_b] = i\epsilon_{abc}B'_c$

Problems

1. Show that the matrices

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

   represent right-hand rotations and can be obtained by cyclicly permuting the rows and columns of any one of them. Note the minus signs.

2. After years of thought and in a moment of inspiration, while walking with his wife on the evening of 1843 October 16, William Rowan Hamilton famously carved into the Brougham Bridge on the Royal Canal in Dublin Ireland the algebra governing three-dimensional rotation combinations.

   (a) The hermitian *and* unitary Pauli spin matrices

$$\{I, \sigma_x, \sigma_y, \sigma_z\} = \left\{ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right\}, \tag{3.59}$$

   span a two-dimensional Hilbert space and are isomorphic to Hamilton's *quaternions* $\{\mathbf{1}, \mathbf{i}, \mathbf{j}, \mathbf{k}\}$. Prove the following identities.

   i. $\sigma_a \sigma_b = -\sigma_b \sigma_a$ (anticommuting).
   ii. $\sigma_a^2 = I$ (unit squares).
   iii. $(\vec{u}\cdot\vec{\sigma})(\vec{v}\cdot\vec{\sigma}) = I\vec{u}\cdot\vec{v} + i\,\vec{u}\times\vec{v}\cdot\vec{\sigma}$ (dot and cross product relation).

   (b) Show geometrically that the rotation of vector $\vec{v}$ about an axis $\hat{\theta}$ through an angle θ is

$$\begin{aligned} \vec{v}\,' &= \vec{v}_\perp \cos\theta + \hat{\theta}\times\vec{v}_\perp \sin\theta + \vec{v}_{\|} \\ &= \left(\vec{v} - \hat{\theta}\left(\hat{\theta}\cdot\vec{v}\right)\right)\cos\theta + \hat{\theta}\times\vec{v}\sin\theta + \hat{\theta}\left(\hat{\theta}\cdot\vec{v}\right). \end{aligned} \tag{3.60}$$

   (c) Expand the vector

$$\vec{v} = v_x\hat{x} + v_y\hat{y} + v_z\hat{z} \tag{3.61}$$

   in Pauli matrices

$$\vec{v}\cdot\vec{\sigma} = v_x\sigma_x + v_y\sigma_y + v_z\sigma_z \tag{3.62}$$

   and show that the Eq. 3.60 rotation is equivalent to

$$\vec{v}\,'\cdot\vec{\sigma} = U_{\vec{\theta}}\,\vec{v}\cdot\vec{\sigma}\,U_{\vec{\theta}}^\dagger = e^{-i\vec{\sigma}\cdot\vec{\theta}/2}\,\vec{v}\cdot\vec{\sigma}\,e^{+i\vec{\sigma}\cdot\vec{\theta}/2}, \tag{3.63}$$

   where the unitary operator

$$U_{\vec{\theta}} = e^{-i\vec{\sigma}\cdot\vec{\theta}/2} = I\cos\frac{\theta}{2} - i\vec{\sigma}\cdot\hat{\theta}\sin\frac{\theta}{2}. \tag{3.64}$$

(d) To combine rotations, simply multiply the Eq. 3.64 unitary transformations, $U_3 = U_2 U_1$, or

$$e^{-i\vec{\sigma}\cdot\vec{\theta}_3/2} = e^{-i\vec{\sigma}\cdot\vec{\theta}_2/2} e^{-i\vec{\sigma}\cdot\vec{\theta}_1/2}. \tag{3.65}$$

Expand and equate real and imaginary parts to show

$$\cos\frac{\theta_3}{2} = \cos\frac{\theta_2}{2}\cos\frac{\theta_1}{2} - \hat{\theta}_2\cdot\hat{\theta}_1 \sin\frac{\theta_2}{2}\sin\frac{\theta_1}{2}, \tag{3.66a}$$

$$\hat{\theta}_3 \sin\frac{\theta_3}{2} = \hat{\theta}_2 \sin\frac{\theta_2}{2}\cos\frac{\theta_1}{2} + \hat{\theta}_1 \cos\frac{\theta_2}{2}\sin\frac{\theta_1}{2} + \hat{\theta}_2\times\hat{\theta}_1 \sin\frac{\theta_2}{2}\sin\frac{\theta_1}{2}. \tag{3.66b}$$

Note that generally $\vec{\theta}_3 \neq \vec{\theta}_2 + \vec{\theta}_1$, but if $\hat{\theta}_1 = \hat{\theta}_2$, then $\theta_3 = \theta_2 + \theta_1$ and $\hat{\theta}_3 = \hat{\theta}_2 = \hat{\theta}_1$.

(e) As an example, use Eq. 3.66 to combine a 90° rotation about the z-axis followed by a 90° rotation about the y-axis, and interpret it graphically.

3. Group theory has important applications to both classical and quantum physics. As an example, the symmetry group of an equilateral triangle consists of 6 operations: A and B rotate 120° and 240° about a line perpendicular to the center, C and D and E reflect about lines through a vertex and the center, and I doesn't change anything. Show that these 6 operations form a group. To demonstrate closure, explicitly construct a 6×6 multiplication table.

4. Prove the "product rule" commutator identity

$$[AB, C] = [A, C]B + A[B, C], \tag{3.67}$$

and compare it to the product differentiation rule $d(fg)/dx$.

5. Verify that the Table 3.2 phase constants φ^8_{ab} is absorbable.

6. Verify that the Table 3.2 phase constants φ^1_{ab}, φ^2_{ab}, and φ^4_{ab} are eliminable.

Chapter 4

Dynamics Commutators

Each symmetry generator corresponds to an observable dynamical variable.

4.1 Position Operator

To associate dynamical operators with the symmetry generators, assume the position operator $\vec{Q}$ has commuting components Q_a with eigenvalues $\vec{x}$ and eigenstates $|\vec{x}\rangle$, so

$$\vec{Q}\,|\vec{x}\rangle = \vec{x}\,|\vec{x}\rangle \tag{4.1}$$

or

$$Q_a\,|\vec{x}\rangle = x_a\,|\vec{x}\rangle \tag{4.2}$$

for $a \in \{1,2,3\}$.

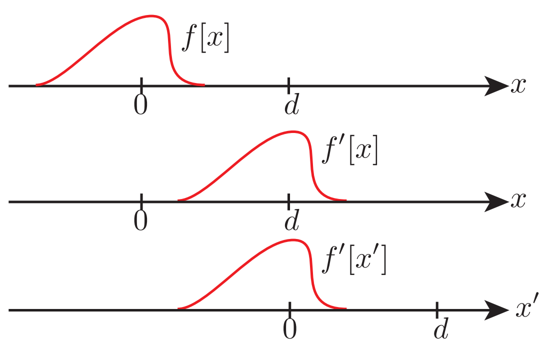


Figure 4.1: A translated function at a translated point is the original function at the original point, $f'[x'] = f[x]$.

Fix sign conventions by assuming, as in Fig. 4.1, that a transformed position eigenstate at a transformed position is the original eigenstate at the original position,

$$|\vec{x}\,'\rangle' = U[\mathcal{T}_{\vec{\epsilon}}]|\mathcal{T}_{\vec{\epsilon}}\,\vec{x}\rangle = |\vec{x}\rangle\,, \tag{4.3}$$

so that

$$U[\mathcal{T}_{\vec{\epsilon}}]|\vec{x}\rangle = \left|\mathcal{T}_{\vec{\epsilon}}^{-1}\,\vec{x}\right\rangle. \tag{4.4}$$

Consequently, the position eigenvalue Eq. 4.1 transforms as

$$U\vec{Q}\,U^{-1}U\,|\vec{x}\rangle = \vec{x}\,U\,|\vec{x}\rangle\,, \tag{4.5a}$$
$$U\vec{Q}U^{-1}\left|\mathcal{T}_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle = \vec{x}\left|\mathcal{T}_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle, \tag{4.5b}$$
$$\vec{Q}'\,|\vec{x}\rangle = \mathcal{T}_{\vec{\epsilon}}\vec{x}\,|\vec{x}\rangle\,, \tag{4.5c}$$

where the position operator transforms like

$$\vec{Q}' = U[\mathcal{T}_{\vec{\epsilon}}]\vec{Q}\,U[\mathcal{T}_{\vec{\epsilon}}]^{-1} = U[\mathcal{T}_{\vec{\epsilon}}]\vec{Q}\,U[\mathcal{T}_{\vec{\epsilon}}]^{\dagger} = e^{i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}\vec{Q}e^{-i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}. \tag{4.6}$$

For small transforms, to $\mathcal{O}[\epsilon]$, this becomes

$$\begin{aligned}\vec{Q}' &= \left(1 + i\vec{\epsilon}\cdot\vec{\mathcal{T}}'\right)\vec{Q}\left(1 - i\vec{\epsilon}\cdot\vec{\mathcal{T}}'\right)\\ &= \vec{Q} + i\vec{\epsilon}\cdot\vec{\mathcal{T}}'\,\vec{Q} - i\vec{Q}\,\vec{\epsilon}\cdot\vec{\mathcal{T}}'\\ &= \vec{Q} + i\left[\vec{\epsilon}\cdot\vec{\mathcal{T}}',\vec{Q}\right],\end{aligned} \tag{4.7}$$

and the mixed commutator of a symmetry generator and a position operator

$$i\left[\vec{\epsilon}\cdot\vec{\mathcal{T}}',\vec{Q}\right] = \vec{Q}' - \vec{Q} = \mathcal{T}_{\vec{\epsilon}}\vec{x}I - \vec{Q}. \tag{4.8}$$

4.1.1 Position and Space Translations

More specifically, under space translations,

$$S_{\vec{\epsilon}}\,\vec{x} = \vec{x} + \vec{\epsilon}, \tag{4.9}$$

the Eq. 4.1 position eigenvalue equation transforms as

$$U\vec{Q}\,U^{-1}U\,|\vec{x}\rangle = \vec{x}\,U\,|\vec{x}\rangle\,, \tag{4.10a}$$
$$U\vec{Q}U^{-1}\left|S_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle = \vec{x}\left|S_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle, \tag{4.10b}$$
$$\begin{aligned}\vec{Q}'\,|\vec{x}\rangle &= S_{\vec{\epsilon}}\,\vec{x}\,|\vec{x}\rangle\\ &= (\vec{x} + \vec{\epsilon})\,|\vec{x}\rangle\\ &= (\vec{Q} + \vec{\epsilon}\,I)\,|\vec{x}\rangle\,,\end{aligned} \tag{4.10c}$$

Since the state $|\vec{x}\rangle$ is arbitrary,

$$\vec{Q}' = \vec{Q} + \vec{\epsilon}\,I. \tag{4.11}$$

But under space translations the position operator also transforms like

$$\vec{Q}' = U[S_{\vec{\epsilon}}]\vec{Q}\,U[S_{\vec{\epsilon}}]^{-1} = e^{i\vec{\epsilon}\cdot\vec{S}'}\vec{Q}e^{-i\vec{\epsilon}\cdot\vec{S}'}, \tag{4.12}$$

which to $\mathcal{O}[\epsilon]$ becomes

$$\begin{aligned}\vec{Q}' &= \left(1 + i\vec{\epsilon}\cdot\vec{S}'\right)\vec{Q}\left(1 - i\vec{\epsilon}\cdot\vec{S}'\right)\\ &= \vec{Q} + i\vec{\epsilon}\cdot\vec{S}'\,\vec{Q} - i\vec{Q}\,\vec{\epsilon}\cdot\vec{S}'\\ &= \vec{Q} + i\left[\vec{\epsilon}\cdot\vec{S}',\vec{Q}\right]. \end{aligned} \tag{4.13}$$

By comparison, the mixed commutator of translation generator and position operator

$$i\left[\vec{\epsilon}\cdot\vec{S}',\vec{Q}\right] = \vec{\epsilon}\,I \tag{4.14}$$

or

$$i\left[\vec{\epsilon}\cdot\vec{S}',Q_a\right] = \epsilon_a I. \tag{4.15}$$

If $\epsilon_a = \epsilon\delta_{ab}$, then

$$i[S_b', Q_a] = \delta_{ab} I \tag{4.16}$$

or

$$[Q_a, S_b'] = i\delta_{ab} I. \tag{4.17}$$

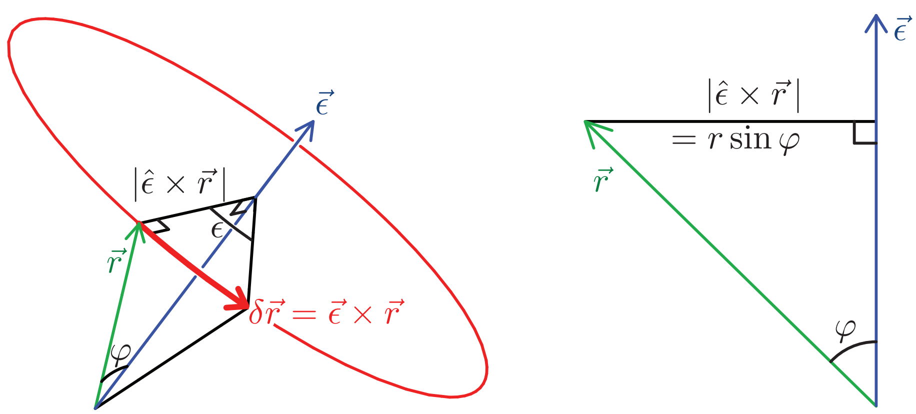


Figure 4.2: Cross product produces an infinitesimal rotation.

4.1.2 Position and Rotations

Under space rotations,

$$R_{\vec{\epsilon}}\,\vec{x} = \vec{x} + \vec{\epsilon}\times\vec{x} + \mathcal{O}[\epsilon^2], \tag{4.18}$$

as in Fig. 4.2, the Eq. 4.1 position eigenvalue equation transforms as

$$U\vec{Q}\,U^{-1}U\,|\vec{x}\rangle = \vec{x}\,U\,|\vec{x}\rangle\,, \tag{4.19a}$$

$$U\vec{Q}U^{-1}\left|R_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle = \vec{x}\left|R_{\vec{\epsilon}}^{-1}\vec{x}\right\rangle, \tag{4.19b}$$

$$\begin{aligned}\vec{Q}'\,|\vec{x}\rangle &= R_{\vec{\epsilon}}\,\vec{x}\,|\vec{x}\rangle \\ &= (\vec{x}+\vec{\epsilon}\times\vec{x})\,|\vec{x}\rangle \\ &= (\vec{Q}+\vec{\epsilon}\times\vec{Q})\,|\vec{x}\rangle\,,\end{aligned} \tag{4.19c}$$

Since the state $|\vec{x}\rangle$ is arbitrary,

$$\vec{Q}' = \vec{Q} + \vec{\epsilon}\times\vec{Q}. \tag{4.20}$$

But under space rotations the position operator also transforms like

$$\vec{Q}' = U[R_{\vec{\epsilon}}]\vec{Q}\,U[R_{\vec{\epsilon}}]^{-1} = e^{i\vec{\epsilon}\cdot\vec{R}'}\vec{Q}e^{-i\vec{\epsilon}\cdot\vec{R}'}, \tag{4.21}$$

which to $\mathcal{O}[\epsilon]$ becomes

$$\begin{aligned}\vec{Q}' &= \left(1+i\vec{\epsilon}\cdot\vec{R}'\right)\vec{Q}\left(1-i\vec{\epsilon}\cdot\vec{R}'\right) \\ &= \vec{Q} + i\vec{\epsilon}\cdot\vec{R}'\,\vec{Q} - i\vec{Q}\,\vec{\epsilon}\cdot\vec{R}' \\ &= \vec{Q} + i\left[\vec{\epsilon}\cdot\vec{R}',\vec{Q}\right].\end{aligned} \tag{4.22}$$

By comparison, the mixed commutator of rotation generator and position operator

$$i\left[\vec{\epsilon}\cdot\vec{R}',\vec{Q}\right] = \vec{\epsilon}\times\vec{Q}. \tag{4.23}$$

Projecting on the vector $\vec{v}$,

$$i\left[\vec{\epsilon}\cdot\vec{R}',\vec{v}\cdot\vec{Q}\right] = \vec{v}\cdot\vec{\epsilon}\times\vec{Q}. \tag{4.24}$$

If $\vec{\epsilon} = \epsilon\hat{x}_a$ and $\vec{v} = v\hat{x}_b$, then

$$i[R'_a, Q_b] = \hat{x}_b\cdot\hat{x}_a\times\vec{Q} = \hat{x}_b\times\hat{x}_a\cdot\vec{Q} = -\epsilon_{abc}\hat{x}_c\cdot\vec{Q} \tag{4.25}$$

or

$$[R'_a, Q_b] = i\epsilon_{abc}Q_c. \tag{4.26}$$

4.1.3 Position and Boosts

Under velocity translations or boosts,

$$B_{\vec{\epsilon}}\vec{x}_t = \vec{x}_t + \vec{\epsilon}t, \tag{4.27}$$

the Eq. 4.1 position eigenvalue equation transforms as

$$U\vec{Q}\,U^{-1}U\,|\vec{x}_t\rangle = \vec{x}_t\,U\,|\vec{x}\rangle\,, \tag{4.28a}$$
$$U\vec{Q}U^{-1}\,\left|B_{\vec{\epsilon}}^{-1}\vec{x}_t\right\rangle = \vec{x}_t\left|B_{\vec{\epsilon}}^{-1}\vec{x}_t\right\rangle, \tag{4.28b}$$
$$\begin{aligned}\vec{Q}'\,|\vec{x}_t\rangle &= B_{\vec{\epsilon}}\,\vec{x}_t\,|\vec{x}_t\rangle \\ &= (\vec{x}_t + \vec{\epsilon}\,t)\,|\vec{x}_t\rangle \\ &= (\vec{Q} + \vec{\epsilon}\,tI)\,|\vec{x}_t\rangle\,,\end{aligned} \tag{4.28c}$$

Since the state $|\vec{x}_t\rangle$ is arbitrary,

$$\vec{Q}' = \vec{Q} + \vec{\epsilon}\,tI. \tag{4.29}$$

But under boosts the position operator also transforms like

$$\vec{Q}' = U[B_{\vec{\epsilon}}]\vec{Q}\,U[B_{\vec{\epsilon}}]^{-1} = e^{i\vec{\epsilon}\cdot\vec{B}'}\vec{Q}e^{-i\vec{\epsilon}\cdot\vec{B}'}, \tag{4.30}$$

which to $\mathcal{O}[\epsilon]$ becomes

$$\begin{aligned}\vec{Q}' &= \left(1 + i\vec{\epsilon}\cdot\vec{B}'\right)\vec{Q}\left(1 - i\vec{\epsilon}\cdot\vec{B}'\right) \\ &= \vec{Q} + i\vec{\epsilon}\cdot\vec{B}'\,\vec{Q} - i\vec{Q}\,\vec{\epsilon}\cdot\vec{B}' \\ &= \vec{Q} + i\left[\vec{\epsilon}\cdot\vec{B}',\vec{Q}\right].\end{aligned} \tag{4.31}$$

By comparison, the mixed commutator of boost generator and position operator

$$i\left[\vec{\epsilon}\cdot\vec{B}',\vec{Q}\right] = \vec{\epsilon}\,tI \tag{4.32}$$

or

$$i\left[\vec{\epsilon}\cdot\vec{B}',Q_a\right] = \epsilon_a tI. \tag{4.33}$$

If $\vec{\epsilon} = \epsilon\delta_{ab}$, then

$$i[B_b',Q_a] = \delta_{ab}tI \tag{4.34}$$

or

$$[Q_a,B_b'] = i\delta_{ab}tI. \tag{4.35}$$

Without loss of generality, at $t = 0$ there is no position change, and

$$[Q_a,B_b'] = 0, \tag{4.36}$$

where $U[B_{\vec{\epsilon}}] = \exp[i\vec{\epsilon}\cdot\vec{B}']$ hereafter describes the instantaneous effects of a velocity translation or boost.

4.1.4 Position and Time Translations

Nonrelativistic quantum mechanics does not treat time and space equally: time t is a parameter while space $\vec{x}$ is associated with the position operator $\vec{Q}$. Hence, discovering the mixed commutator of the time translation generator and the position operators requires a different technique.

Under time translations,

$$T_\epsilon \vec{x}_t = \vec{x}_{t+\epsilon}, \tag{4.37}$$

in order for the new state at the new time to be the old state at the old time,

$$|\psi_{t'}\rangle' = U[T_\epsilon]\big|\psi_{T_\epsilon t}\big\rangle = |\psi_t\rangle. \tag{4.38}$$

then the new state at the old time

$$|\psi_t\rangle' = e^{i\epsilon T'}|\psi_t\rangle = U[T_\epsilon]|\psi_t\rangle = \big|\psi_{T_\epsilon^{-1}t}\big\rangle = |\psi_{t-\epsilon}\rangle. \tag{4.39}$$

If $\epsilon = t$, then

$$e^{itT'}|\psi_t\rangle = |\psi_0\rangle. \tag{4.40}$$

and

$$|\psi_t\rangle = e^{-itT'}|\psi_0\rangle. \tag{4.41}$$

Differentiate both sides with respect to the time t parameter to find

$$\frac{|\psi_{t+dt}\rangle - |\psi_t\rangle}{dt} = \frac{d}{dt}|\psi_t\rangle = -iT'|\psi_t\rangle \tag{4.42}$$

and its adjoint

$$\frac{\langle\psi_{t+dt}| - \langle\psi_t|}{dt} = \frac{d}{dt}\langle\psi_t| = \langle\psi_t|iT'. \tag{4.43}$$

4.2 Velocity Operator

Introduce the *velocity* operator by the classical correspondence of expectation values

$$\left\langle \vec{V} \right\rangle = \frac{d}{dt}\left\langle \vec{Q} \right\rangle \tag{4.44}$$

or, more explicitly,

$$\begin{aligned}
\left\langle \psi_t \middle| \vec{V} \middle| \psi_t \right\rangle &= \frac{d}{dt}\left\langle \psi_t \middle| \vec{Q} \middle| \psi_t \right\rangle \\
&= \left(\frac{d}{dt}\langle\psi_t|\right)\vec{Q}\,|\psi_t\rangle + \langle\psi_t|\,\vec{Q}\left(\frac{d}{dt}|\psi_t\rangle\right) \\
&= \langle\psi_t|\,iT'\vec{Q}\,|\psi_t\rangle - \langle\psi_t|\,i\vec{Q}T'\,|\psi_t\rangle \\
&= \langle\psi_t|\,i\left[T', \vec{Q}\right]|\psi_t\rangle\,.
\end{aligned} \tag{4.45}$$

Since this is true for all state vectors,

$$\vec{V} = i\left[T', \vec{Q}\right] \tag{4.46}$$

or

$$[Q_a, T'] = iV_a. \tag{4.47}$$

Compute the mixed commutators of the velocity operator with the symmetry generators using the Section 4.1 position operator techniques or by the antisymmetry of the existing commutators. For example,

$$\begin{aligned}
\left[\vec{\epsilon}\cdot\vec{B}', V_b\right] &= \epsilon_a[B'_a, V_b] \\
&= -i\epsilon_a[B'_a, [Q_b, T']] \\
&= i\epsilon_a\big([T', [B'_a, Q_b]] + [Q_b, [T', B'_a]]\big) \\
&= i\epsilon_a\big([T', 0] - i[Q_b, S'_a]\big) \\
&= i\epsilon_a(0 + \delta_{ba}I) \\
&= i\epsilon_b I
\end{aligned} \tag{4.48}$$

with $\vec{\epsilon} = \epsilon\hat{x}_a$ implies

$$[B'_a, V_b] = i\delta_{ab}I. \tag{4.49}$$

Note that the boost of the velocity operator is

$$\begin{aligned}
U[B_{\vec{\epsilon}}]\vec{V}\,U[B_{\vec{\epsilon}}]^{-1} &= e^{i\vec{\epsilon}\cdot\vec{B}'}\vec{V}e^{-i\vec{\epsilon}\cdot\vec{B}'} \\
&= \left(1 + i\vec{\epsilon}\cdot\vec{B}'\right)\vec{V}\left(1 - i\vec{\epsilon}\cdot\vec{B}'\right) \\
&= \vec{V} + i\vec{\epsilon}\cdot\vec{B}'\,\vec{V} - i\vec{V}\,\vec{\epsilon}\cdot\vec{B}' \\
&= \vec{V} + i\left[\vec{\epsilon}\cdot\vec{B}', \vec{V}\right] \\
&= \vec{V} - \vec{\epsilon}I
\end{aligned} \tag{4.50}$$

to $\mathcal{O}[\epsilon]$ (and by Eq. 4.113, this is true to all orders of ϵ). As a consequence, the operator transformation

$$\vec{V}' = e^{i\vec{\epsilon}\cdot\vec{B}'}\vec{V}e^{-i\vec{\epsilon}\cdot\vec{B}'} = \vec{V} - \vec{\epsilon}I, \tag{4.51}$$

which is plausible, as boosts are velocity translations.

Table 4.1 summarizes the commutations relations of the position and velocity operators with the Galilei symmetry generators for free particles, while Table 4.2 summarizes the infinitesimal transformations of states and observables.

Table 4.1: Mixed commutators of position and velocity operators with the free particle symmetry generators representing Galilei transformations.

$[Q_a, T'] = iV_a$	$[V_a, T'] = 0$
$[Q_a, S'_b] = i\delta_{ab}I$	$[V_a, S'_b] = 0$
$[Q_a, R'_b] = i\epsilon_{abc}Q_c$	$[V_a, R'_b] = -i\epsilon_{abc}V_c$
$[Q_a, B'_b] = 0$	$[V_a, B'_b] = -i\delta_{ab}I$

Table 4.2: Infinitesimal Hilbert space transformations of states (vectors) and observables (operators) corresponding to Galilei real space transformations.

operation	$\vec{\mathcal{T}}'$	$e^{i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}\lvert\psi_t[\vec{x}]\rangle$	$e^{i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}\vec{Q}e^{-i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}$	$e^{i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}\vec{V}e^{-i\vec{\epsilon}\cdot\vec{\mathcal{T}}'}$
time translations	T'	$\lvert\psi_{t-\epsilon}[\vec{x}]\rangle$	$\vec{Q}+\vec{V}\epsilon$	$\vec{V}$
space translations	$\vec{S}'$	$\lvert\psi_t[\vec{x}-\vec{\epsilon}]\rangle$	$\vec{Q}+\vec{\epsilon}\,I$	$\vec{V}$
space rotations	$\vec{R}'$	$\lvert\psi_t[\vec{x}-\vec{\epsilon}\times\vec{x}]\rangle$	$\vec{Q}+\vec{\epsilon}\times\vec{Q}$	$\vec{V}+\vec{\epsilon}\times\vec{V}$
instant boosts	$\vec{B}'$	$\lvert\psi_t[\vec{x}]\rangle$	$\vec{Q}$	$\vec{V}-\vec{\epsilon}\,I$

4.3 Symmetry Generators Dynamical Identities

The preceding commutation relations suffice to associate each generator with a dynamical operator.

4.3.1 Free Particle Without Spin

Introduction

The consistency of Tables 3.3 & 4.1 suggests that boost generators are proportional to position operators, $\vec{B}' \propto \vec{Q}$. Identifying boost generators with position operators $\hbar B'_a = MQ_a$ implies

$$i\delta_{ab}I = [Q_a, S'_b] = \hbar[B'_a, S'_b]/M = \hbar\, i\delta_{ab}\mu I/M \tag{4.52}$$

which itself implies that the particle's mass

$$M = \mu\hbar, \tag{4.53}$$

where $\hbar$ (pronounced "h-bar") is a dimensional constant. The Table 4.1 position time translation commutator then identifies space translation generators with momentum operators,

$$P_a = MV_a = -i[MQ_a, T'] = -i[\hbar B'_a, T'] = -i\hbar\, iS'_a = \hbar S'_a. \tag{4.54}$$

This obvious first identification,

$$\hbar\vec{B}' = M\vec{Q} \equiv \vec{C}, \tag{4.55a}$$

$$\hbar\vec{S}' = M\vec{V} \equiv \vec{P}, \tag{4.55b}$$

and Table 4.1 implies the famous position-momentum commutator

$$[Q_a, P_b] = i\hbar\delta_{ab}I, \tag{4.56}$$

which implies (in popular notation)

$$[X, P_x] = i\hbar. \tag{4.57}$$

Irreducible Sets

For a particle with no internal degrees of freedom, the position and momentum operators $\{\vec{Q}, \vec{P}\}$ are *irreducible*: if an operator commutes with $\vec{Q}$, it cannot be a function of $\vec{P}$, and if it commutes with $\vec{P}$, it cannot be a function of $\vec{Q}$, and if it commutes with both $\vec{Q}$ and $\vec{P}$, it must be a constant. This is plausible physically, as classical Hamiltonian dynamics uniquely determines orbits based on single initial points in position-momentum "phase space". The Eq. 4.55 identification thus implies that the generators of velocity and space translations $\{\vec{B}', \vec{S}'\}$ are also irreducible.

Position

Assuming $\{\vec{B}', \vec{S}'\}$ irreducibility, check that the identification of boost generators with position operators is unique by noting that since $\hbar\vec{B}' - M\vec{Q}$ commutes with space translation generators $\vec{S}'$,

$$\begin{aligned}[\hbar B'_a - MQ_a, S'_b] &= \hbar[B'_a, S'_b] - M[Q_a, S'_b] \\ &= \cancel{\hbar i\delta_{ab}\mu I} - \cancel{Mi\delta_{ab}I} = 0,\end{aligned} \tag{4.58}$$

assuming $M = \mu\hbar$, it cannot be a function of $\vec{S}'$. Since it commutes with velocity translation generators $\vec{B}'$,

$$[\hbar B'_a - MQ_a, B'_b] = \hbar[B'_a, B'_b] - M[Q_a, B'_b] = 0 - 0 = 0, \tag{4.59}$$

it cannot be a function of $\vec{B}'$. Thus, if there are no internal degrees of freedom, it must be a constant,

$$\hbar\vec{B}' - M\vec{Q}_a = \vec{k}I. \tag{4.60}$$

But from Table 4.1,

$$[R'_a, Q_b] = i\epsilon_{abc}Q_c, \tag{4.61a}$$

$$[R'_a, MQ_b] = i\epsilon_{abc}MQ_c, \tag{4.61b}$$

$$[R'_a, \hbar B'_b - k_bI] = i\epsilon_{abc}(\hbar B'_c - k_cI), \tag{4.61c}$$

$$\cancel{\hbar[R'_a, B'_b]} = \cancel{\hbar i\epsilon_{abc}B'_c} - i\epsilon_{abc}k_cI, \tag{4.61d}$$

so the constant $\vec{k} = \vec{0}$.

Linear Momentum

Still assuming $\{\vec{B}', \vec{S}'\}$ irreducibility, check that the identification of space translation generators with momentum operators is unique by noting that since $\hbar\vec{S}' - \vec{P}$ commutes with space translation generators $\vec{S}'$,

$$[\hbar S'_a - P_a, S'_b] = \hbar[S'_a, S'_b] - M[V_a, S'_b] = 0 - 0 = 0, \tag{4.62}$$

it cannot be a function of $\vec{S}'$. Since it commutes with velocity translation generators $\vec{B}'$,

$$[\hbar S'_a - P_a, B'_b] = \hbar[S'_a, B'_b] - M[V_a, B'_b] = \hbar(-i\delta_{ab}\mu I) + M\, i\hbar\delta_{ab}I = 0, \tag{4.63}$$

as $M = \mu\hbar$, it cannot be a function of $\vec{B}'$. Thus, if there are no internal degrees of freedom, it must be a constant,

$$\hbar\vec{S}' - \vec{P} = \vec{k}I. \tag{4.64}$$

But from Table 4.1,

$$\begin{aligned}
i\epsilon_{abc}S'_c &= [R'_a, S'_b], && (4.65a)\\
i\epsilon_{abc}\hbar S'_c &= [R'_a, \hbar S'_b], && (4.65b)\\
i\epsilon_{abc}(MV_c + k_cI) &= [R'_a, MV_b + k_bI], && (4.65c)\\
\cancel{i\epsilon_{abc}MV_c} + i\epsilon_{abc}k_cI &= M[R'_a, V_b],\\
&= -iM[R'_a, [Q_b, T']]\\
&= iM([T', [R'_a, Q_b]] + [Q_b, [T', R'_a]])\\
&= -\epsilon_{abc}M([T', Q_c] + [Q_b, 0])\\
&= \cancel{i\epsilon_{abc}MV_c}, && (4.65d)
\end{aligned}$$

so the constant $\vec{k} = \vec{0}$.

Angular Momentum

Furthermore, identifying rotation generators with angular momenta operators $\hbar R'_a = \epsilon_{abc}Q_bP_c = L_c$ implies

$$\begin{aligned}
\cancel{[R'_a, B'_b]} &= \epsilon_{acd}[Q_cP_d, B'_b]/\hbar\\
&= \epsilon_{acd}[B'_cS'_d, B'_b]\hbar/M\\
&= \epsilon_{acd}(B'_c[S'_d, B'_b] + [B'_c, B'_b]S'_d)\hbar/M\\
&= \epsilon_{acd}(-i\delta_{bd}\mu B'_c + 0)\hbar/M\\
&= -i\epsilon_{acb}B'_c\\
&= \cancel{i\epsilon_{abc}B'_c}, && (4.66)
\end{aligned}$$

and similarly for the other Table 3.3 blue commutators. Now $\{\vec{B}', \vec{S}'\}$ irreducibility implies $\{\vec{Q}, \vec{P}\}$ irreducibility, so check that this identification is necessary by noting that since $\hbar R'_a - \epsilon_{abc} Q_b P_c$ commutes with momentum $\vec{P}$,

$$\begin{aligned}[\hbar R'_a - \epsilon_{abc} Q_b P_c, P_b] &= \hbar[R'_a, P_b] - \epsilon_{abc}[Q_b P_c, P_b] \\ &= \hbar^2 [R'_a, S'_b] - \epsilon_{abc}(Q_b [P_c, P_b] + [Q_b, P_b] P_c) \\ &= \hbar^2 i\epsilon_{abc} S'_c - \epsilon_{abc} i\hbar P_c = 0, \end{aligned} \tag{4.67}$$

it cannot be a function of $\vec{P}$. Since it commutes with position $\vec{Q}$,

$$\begin{aligned}[\hbar R'_a - \epsilon_{abc} Q_b P_c, Q_b] &= \hbar[R'_a, Q_b] - i\epsilon_{abc}[Q_b P_c, Q_b] \\ &= \hbar i\epsilon_{abc} Q_c - i\epsilon_{abc}(Q_b [P_c, Q_b] + [Q_b, Q_b] P_c) \\ &= -\hbar i\epsilon_{abc} Q_b + \epsilon_{abc} i\hbar Q_b = 0, \end{aligned} \tag{4.68}$$

it cannot be a function of $\vec{Q}$. Thus, if there are no internal degrees of freedom, it must be a constant,

$$\hbar R'_a - \epsilon_{abc} Q_b P_c = k_a I. \tag{4.69}$$

But from Tables 3.3 & 4.1 and the Eq. 4.111b identity,

$$\begin{aligned} [R'_a, R'_b] &= i\epsilon_{abc} R'_c, \\ [\hbar R'_a, R'_b] &= i\epsilon_{abc} \hbar R'_c, \\ [\epsilon_{acd} Q_c P_d + k_a I, R'_b] &= i\epsilon_{abc}(\epsilon_{cde} Q_d P_e + k_c I), \\ \epsilon_{acd} \hbar^2 [B'_c S'_d, R'_b] &= i\epsilon_{abc} \hbar^2 (\epsilon_{cde} B'_d S'_e + M k_c I), \\ \epsilon_{acd}(B'_c [S'_d, R'_b] + [B'_c, R'_b] S'_d) &= i\epsilon_{abc}\epsilon_{cde} B'_d S'_e + i\epsilon_{abc} M k_c / I\hbar^2, \\ \epsilon_{acd}(-i\epsilon_{bde} B'_c S'_e - i\epsilon_{bce} B'_e S'_d) &= i(\delta_{ad}\delta_{be} - \delta_{ae}\delta_{bd}) B'_d S'_e + i\epsilon_{abc} M k_c I/\hbar^2, \\ \epsilon_{dac}\epsilon_{dbe} B'_c S'_e - \epsilon_{cad}\epsilon_{cbe} B'_e S'_d &= (\delta_{ad}\delta_{be} - \delta_{ae}\delta_{bd}) B'_d S'_e + \epsilon_{abc} M k_c I/\hbar^2, \\ (\delta_{ab}\delta_{ce} - \delta_{ae}\delta_{cb}) B'_c S'_e - (\delta_{ab}\delta_{de} - \delta_{ae}\delta_{db}) B'_e S'_d &= B'_a S'_b - B'_b S'_a + \epsilon_{abc} M k_c I/\hbar^2, \\ \delta_{ab} \vec{B}' \cdot \vec{S}' - B'_b S'_a - \delta_{ab} \vec{B}' \cdot \vec{S}' + B'_a S'_b &= B'_a S'_b - B'_b S'_a + \epsilon_{abc} M k_c I/\hbar^2, \\ 0 &= \epsilon_{abc} M k_c I/\hbar^2, \end{aligned} \tag{4.70}$$

so the constant $\vec{k} = \vec{0}$.

Energy

Finally, identifying time translation generators with the energy operator $\hbar T' = P_a P_a / 2M = H$ implies

$$\begin{aligned}[B'_a, T'] &= [B'_a, P_b P_b]/2M\hbar \\ &= [B'_a, S'_b S'_b]\hbar/2M \\ &= (S'_b [B'_a, S'_b] + [B'_a, S'_b] S'_b)\hbar/2M \\ &= (S'_b\, i\delta_{ab}\mu I + i\delta_{ab}\mu I\, S'_b)\hbar/2M \\ &= iS'_a. \end{aligned} \tag{4.71}$$

Again assuming $\{\vec{Q},\vec{P}\}$ irreducibility, check that this identification is unique by noting that since $\hbar T' - P_a P_a/2M$ commutes with momentum P_b,

$$\begin{aligned}[\hbar T' - P_a P_a/2M, P_b] &= \hbar[T', P_b] - [P_a P_a, P_b]/2M \\ &= \hbar[T', S'_b] - P_a[P_a, P_a]/2M - [P_a, P_a]P_a/2M \\ &= 0 - 0 - 0 = 0, \end{aligned} \tag{4.72}$$

it cannot be a function of Q_a. Since it commutes with position Q_a,

$$\begin{aligned} 2M[\hbar T' - P_b P_b/2M, Q_b] &= 2M\hbar[T', Q_b] - [P_a P_a, Q_b] \\ &= 2\hbar^2[T', B'_b] - \hbar^3 S'_a[S'_a, B'_b]/M - \hbar^3[S'_a, B'_b]S'_a/M \\ &= -2\hbar^2 i S'_b + S'_b i\delta_{ab}\hbar^3\mu/M + S'_b i\delta_{ab}\hbar^3\mu/M \\ &= -\cancel{2S'_b i\hbar^2} + \cancel{2S'_b i\hbar^2} = 0, \end{aligned} \tag{4.73}$$

it cannot be a function of P_a. Thus, if there are no internal degrees of freedom, it must be a constant,

$$\hbar T' - \frac{P_a P_a}{2M} = E_0 I, \tag{4.74}$$

or

$$\hbar T' = \frac{\vec{P}\cdot\vec{P}}{2M} + E_0 I, \tag{4.75}$$

where E_0 is *undetermined* by the symmetries, but reflects the familiar freedom to choose the zero of energy.

Recap

The simplest identification of generators with dynamical operators that satisfy the commutation relations in vector form is

$$\hbar T' = \tfrac{1}{2}M\vec{V}\cdot\vec{V} \equiv H, \tag{4.76a}$$
$$\hbar \vec{S}' = M\vec{V} \equiv \vec{P}, \tag{4.76b}$$
$$\hbar \vec{R}' = \vec{Q}\times M\vec{V} \equiv \vec{L}, \tag{4.76c}$$
$$\hbar \vec{B}' = M\vec{Q} \equiv \vec{C}, \tag{4.76d}$$

where H is the Hamiltonian energy, $\vec{P}$ is the momentum, $\vec{L}$ is the angular momentum, and $\vec{C} = \sum M_n \vec{Q}_n$ is proportional to the center-of-mass in the multiple particle generalization. The identification in component form is

$$\hbar T' = H = P_a P_a/2M, \tag{4.77a}$$
$$\hbar S'_a = P_a = MV_a, \tag{4.77b}$$
$$\hbar R'_a = L_a = \epsilon_{abc} Q_b P_c, \tag{4.77c}$$
$$\hbar B'_a = C_a = MQ_a, \tag{4.77d}$$

where the Hamiltonian energy $H = \hbar T'$ generates time translations, the linear momentum $\vec{P} = \hbar\vec{S}'$ generates space translations, the angular momentum

$\vec{L} = \hbar\vec{R}'$ generates space rotations, the center-of-mass $\vec{C} = M\vec{Q}$ generates velocity translations or boosts, and the proportionality constant $\hbar$ fixes $M = \mu\hbar$ to be the free particle's mass. Experimentally, *Planck's constant*

$$h = 2\pi\hbar \approx 6.6 \times 10^{-34} \text{ J s} = 0.66 \frac{\text{zJ}}{\text{THz}} \tag{4.78}$$

is (for example) the rate of change of photon energy with frequency. The final dynamical commutation relations, summarized by Table 4.3, form a *Lie* (pronounced "lee") *algebra*.

Table 4.3: Nontrivial dynamical commutators for a free particle without spin.

$[P_a, P_b] = 0$	$[L_a, H] = 0$	$[L_a, L_b] = i\hbar\,\epsilon_{abc}L_c$
$[Q_a, Q_b] = 0$	$[P_a, H] = 0$	$[L_a, P_b] = i\hbar\,\epsilon_{abc}P_c$
$[Q_a, P_b] = i\hbar\,\delta_{ab}I$	$[Q_a, H] = i\hbar P_a/M$	$[L_a, Q_b] = i\hbar\,\epsilon_{abc}Q_c$

4.3.2 Interacting Particles Without Spin

Interactions modify a state's time evolution, invalidating the Table 3.3 symmetry generators involving time. Consequently, redefine $\hbar T' = H$ to be the generator of *dynamic* time evolution, rather than merely *geometric* time translation. However, still constrain time evolution by the independent velocity operator definition

$$\left\langle \vec{V} \right\rangle = \frac{d}{dt}\left\langle \vec{Q} \right\rangle \tag{4.44 reminder}$$

and the resulting commutator

$$[Q_a, T'] = iV_a \tag{4.47 reminder}$$

and operator transform

$$\vec{V} - \vec{\epsilon} I = e^{i\vec{\epsilon}\cdot\vec{B}'}\vec{V}e^{-i\vec{\epsilon}\cdot\vec{B}'}. \tag{4.51 reminder}$$

With interactions, boost generators still correspond to position operators, $\hbar\vec{B}' = M\vec{Q}$, because its derivation does not involve the symmetry generators involving time. Space translation generators still correspond to momentum operators, but the relationship with velocities is generalized. Since $\hbar\vec{S}' - M\vec{V}$ commutes with $\vec{Q}$,

$$\begin{aligned}[\hbar S'_a - MV_a, Q_b] &= \hbar[S'_a, Q_b] - M[V_a, Q_b] \\ &= \hbar[S'_a, B'_b]/M - \hbar[V_a, B'_b] \\ &= -i\delta_{ab}\mu\hbar I/M + \hbar\delta_{ab}I \\ &= 0, \end{aligned} \tag{4.79}$$

and there are no internal degrees of freedom, it must be a function of $\vec{Q}$,

$$\hbar\vec{S}' - M\vec{V} = \vec{A}\left[\vec{Q}\right] \tag{4.80}$$

or

$$\vec{P} \equiv \hbar\vec{S}' = M\vec{V} + \vec{A}\left[\vec{Q}\right], \tag{4.81}$$

where $\vec{A}$ represents momentum stored in the interacting fields.

Similarly, the time translation generator still corresponds to the Hamiltonian energy operator but in a generalized way. Since $\vec{A}$ and $\vec{Q}$ commute, identifying time translation generators with the energy operator

$$\vec{H} \equiv \hbar T' = \left(\vec{P} - \vec{A}\right)^2/2M \tag{4.82}$$

implies

$$\begin{aligned} i[H, Q_a] &= i[(P_b - Q_b)(P_b - Q_b), Q_a]/2M \\ &= i\left([P_b P_b, Q_a] - [P_b A_b, Q_a] - [A_b P_b, Q_a] + [A_b A_b, Q_a]\right)/2M \\ &= i\left(P_b\,[P_b, Q_a] + [P_b, Q_a]\,P_b - [P_b, Q_a]\,A_b - A_b\,[P_b, Q_a] + 0\right)/2M \\ &= i\left(-P_b\,i\hbar\delta_{ab} - i\hbar\delta_{ab}P_b + i\hbar\delta_{ab}A_b + A_b\,i\hbar\delta_{ab}\right)/2M \\ &= (P_a - A_a)/M \\ &= V_a. \end{aligned} \tag{4.83}$$

However, this identification is not unique, as adding or subtracting any function of position $\mathcal{V}[\vec{Q}]$ also works. With the most general identification allowed by the Galilei group of symmetry transformations, external fields shift the free energy and linear momentum operators by functions of position, so

$$H - \mathcal{V}\left[\vec{Q}\right] = \frac{1}{2M}\left(\vec{P} - \vec{\mathcal{A}}\left[\vec{Q}\right]\right)^2. \tag{4.84}$$

4.3.3 Free Particle With Spin

The internal degrees of freedom are independent of position $\vec{Q}$ and momentum $\vec{P}$. In particular, *spin* degrees of freedom generalize the relation between space rotation generators and angular momentum operators to

$$\vec{J} = \vec{L} + \vec{\mathscr{S}}, \tag{4.85}$$

where the spin angular momentum operators satisfy

$$[\mathscr{S}_a, \mathscr{S}_b] = i\epsilon_{abc}\mathscr{S}_c, \tag{4.86}$$

and $\mathscr{S}$ is pronounced “big script s”. The other identifications proceed similarly.

4.4 Position Space Schrödinger Equation

Assuming a time translated state at a time translated instant is the original state at the original instant,

$$|\psi_t'\rangle' = U[T_\epsilon]|\psi_{T_\epsilon t}\rangle = |\psi_t\rangle\,, \tag{4.87}$$

the infinitesimal time translation of a generic state

$$e^{i\epsilon H/\hbar}|\psi_t\rangle = e^{i\epsilon T'}|\psi_t\rangle = U[T_\epsilon]|\psi_t\rangle = \left|\psi_{T_\epsilon^{-1}t}\right\rangle = \left|\psi_{t-\epsilon}\right\rangle \tag{4.88}$$

or

$$\left|\psi_{t-\epsilon}\right\rangle = e^{i\epsilon H/\hbar}|\psi_t\rangle, \tag{4.89}$$

To $\mathcal{O}[\epsilon]$,

$$\left|\psi_{t-\epsilon}\right\rangle = \left(1 + i\epsilon\frac{H}{\hbar}\right)|\psi_t\rangle \tag{4.90}$$

implies the differential equation

$$-i\frac{H}{\hbar}|\psi_t\rangle = \frac{|\psi_t\rangle - |\psi_{t-\epsilon}\rangle}{\epsilon} = \frac{\partial}{\partial t}|\psi_t\rangle \tag{4.91}$$

or

$$H\,|\psi_t\rangle = i\hbar\,\partial_t\,|\psi_t\rangle\,, \tag{4.92}$$

which is the *state space Schrödinger equation*. Since the state $|\psi_t\rangle$ is arbitrary, the Hamiltonian energy operator acts like the time derivative

$$H = +i\hbar\,\partial_t. \tag{4.93}$$

Assuming a space translated position eigenstate at a space translated position is the original eigenstate at the original position,

$$|\vec{x}\,'\rangle' = U[S_{\vec{\epsilon}}]|S_{\vec{\epsilon}}\,\vec{x}\rangle = |\vec{x}\rangle\,, \tag{4.94}$$

the infinitesimal space translation of a position eigenstate

$$e^{i\vec{\epsilon}\cdot\vec{P}/\hbar}|\vec{x}\rangle = e^{i\vec{\epsilon}\cdot\vec{S}'}|\vec{x}\rangle = U[S_{\vec{\epsilon}}]|\vec{x}\rangle = |S_{\vec{\epsilon}}^{-1}\vec{x}\rangle = |\vec{x}-\vec{\epsilon}\rangle. \tag{4.95}$$

and its adjoint

$$\langle\vec{x}-\vec{\epsilon}| = \langle\vec{x}|e^{-i\vec{\epsilon}\cdot\vec{P}/\hbar} \tag{4.96}$$

projected onto a generic state

$$\langle\vec{x}-\vec{\epsilon}|\psi_t\rangle = \langle\vec{x}|e^{-i\vec{\epsilon}\cdot\vec{P}/\hbar}|\psi_t\rangle \tag{4.97}$$

or

$$\psi_t[\vec{x}-\vec{\epsilon}] = e^{-i\vec{\epsilon}\cdot\vec{P}/\hbar}\psi_t[\vec{x}], \tag{4.98}$$

where the operators P_a on state space and the corresponding operators Π_a on wave function space are identified $P_a \leftrightarrow \Pi_a$ by $\langle \vec{x}|P_a|\psi_t\rangle = \Pi_a\langle \vec{x}|\psi_t\rangle$. To $\mathcal{O}[\epsilon]$,

$$\psi_t[\vec{x}-\vec{\epsilon}] = \left(1 - i\vec{\epsilon}\cdot\frac{\vec{P}}{\hbar}\right)\psi_t[\vec{x}] \tag{4.99}$$

implies the differential equation

$$i\hat{\epsilon}\cdot\frac{\vec{P}}{\hbar}\psi_t[\vec{x}] = \frac{\psi_t[\vec{x}]-\psi_t[\vec{x}-\vec{\epsilon}]}{\epsilon} = \hat{\epsilon}\cdot\vec{\nabla}\psi_t[\vec{x}]. \tag{4.100}$$

Since the direction $\hat{\epsilon}$ is arbitrary,

$$\vec{P}\psi_t[\vec{x}] = -i\hbar\vec{\nabla}\psi_t[\vec{x}], \tag{4.101}$$

and since the wave function $\psi_t[\vec{x}]$ is arbitrary, the position representation of the momentum operator acts like the space derivative or gradient

$$\vec{P} = -i\hbar\vec{\nabla}. \tag{4.102}$$

The position operator definition

$$\vec{Q}|\vec{x}\rangle = \vec{x}|\vec{x}\rangle \tag{4.103}$$

and its adjoint

$$\langle\vec{x}|\vec{Q} = \langle\vec{x}|\vec{x} \tag{4.104}$$

projected onto a generic state

$$\langle\vec{x}|\vec{Q}|\psi_t\rangle = \langle\vec{x}|\vec{x}|\psi_t\rangle \tag{4.105}$$

implies

$$\vec{Q}\psi_t[\vec{x}] = \vec{x}\,\psi_t[\vec{x}], \tag{4.106}$$

where again state and wave function operators are identified $Q_a \leftrightarrow \Theta_a$ by $\langle\vec{x}|Q_a|\psi_t\rangle = \Theta_a\langle\vec{x}|\psi_t\rangle$. Since the wave function $\psi_t[\vec{x}]$ is arbitrary, the position representation of the position operator (unsurprisingly) acts like multiplication by position

$$\vec{Q} = \vec{x}. \tag{4.107}$$

Finally, "sandwich" the $\vec{\mathcal{A}} = \vec{0}$ Eq. 4.84 Hamiltonian

$$H = \frac{1}{2M}\vec{P}\cdot\vec{P} + \mathcal{V}[\vec{Q}] \tag{4.108}$$

between the position eigenstate $\langle\vec{x}|$ and the state $|\psi_t\rangle$ to write

$$\langle\vec{x}|H|\psi_t\rangle = \left\langle\vec{x}\left|\tfrac{1}{2M}\vec{P}\cdot\vec{P} + \mathcal{V}[\vec{Q}]\right|\psi_t\right\rangle \tag{4.109}$$

and use the Eq. 4.93, Eq. 4.102, and Eq. 4.107 position representations to write the *position space Schrödinger equation*

$$i\hbar\,\partial_t\psi_t[\vec{x}] = -\frac{\hbar^2}{2M}\nabla^2\psi_t[\vec{x}] + \mathcal{V}[\vec{x}]\psi_t[\vec{x}]. \tag{4.110}$$

Problems

1. Prove the following ϵ-δ identities, with implied sums over repeated indices,

$$\begin{aligned}
\epsilon_{abc}\epsilon_{mno} &= \det \begin{vmatrix} \delta_{am} & \delta_{an} & \delta_{ao} \\ \delta_{bm} & \delta_{bn} & \delta_{bo} \\ \delta_{cm} & \delta_{cn} & \delta_{co} \end{vmatrix} \\
&= +\delta_{am}\delta_{bn}\delta_{co} + \delta_{ao}\delta_{bm}\delta_{cn} + \delta_{an}\delta_{bo}\delta_{cm} \\
&\quad - \delta_{am}\delta_{bo}\delta_{cn} - \delta_{an}\delta_{bm}\delta_{co} - \delta_{ao}\delta_{bn}\delta_{cm}, && (4.111a) \\
\epsilon_{sab}\epsilon_{smn} &= \delta_{am}\delta_{bn} - \delta_{an}\delta_{bm}, && (4.111b) \\
\epsilon_{rsa}\epsilon_{rsm} &= 2\delta_{am}, && (4.111c) \\
\epsilon_{rst}\epsilon_{rst} &= 6, && (4.111d)
\end{aligned}$$

   and use one of them to prove the "bac-cab" identity

$$\vec{a} \times \big(\vec{b} \times \vec{c}\big) = \vec{b}\big(\vec{a} \cdot \vec{c}\big) - \vec{c}\big(\vec{a} \cdot \vec{b}\big). \tag{4.112}$$

2. Prove that $[U_a, U_b] = i\epsilon_{abc}W_c$ is equivalent to $\vec{U} \times \vec{U} = i\vec{W}$.

3. If A and B are operators and x is a parameter, prove that

$$e^{xA}Be^{-xA} = B + [A,B]x + \frac{1}{2!}[A,[A,B]]x^2 + \frac{1}{3!}[A,[A,[A,B]]]x^3 + \cdots . \tag{4.113}$$

   (Hint: If $f[x] = e^{xA}Be^{-xA}$, then show $df/dx = [A, f]$, and so on.)

4. Use Eq. 4.113 to verify the Table 4.2 operator transformations.

5. Substitute the Eq. 4.76 identifications into the Table 4.1 mixed commutators, and show they are consistent with the Table 4.3 final commutators.

6. Compare and contrast the hermitian boost generators $\vec{B}'$ and

$$\hbar\vec{\mathscr{B}}' = M\vec{Q} - t\vec{P}. \tag{4.114}$$

   In particular, use Eq. 4.113 to compute the effects of the corresponding unitary transformations on the position and momentum operators $\vec{Q}$ and $\vec{P}$. Why are boosts also known as velocity translations?

7. Prove the Eq. 4.57 position-momentum commutator in the position basis using the Eq. 4.102 momentum operator representation. (Hint: Apply the commutator to the generic wave function $\psi_t[x]$ and use calculus.)

8. By Eq. 4.102, the momentum acts like a derivative in the position basis,

$$\langle x|P_x|\psi\rangle = -i\hbar\,\partial_x\psi[x] = -i\hbar\,\partial_x\langle x|\psi\rangle. \tag{4.115}$$

(a) Consider $|\psi\rangle = |p\rangle$ to be a state of definite momentum $P_x|p\rangle = p|p\rangle$ and solve

$$\langle x|P_x|p\rangle = -i\hbar\,\partial_x\langle x|p\rangle \tag{4.116}$$

to find

$$\langle x|p\rangle = Ce^{ipx/\hbar}. \tag{4.117}$$

(b) To find the constant C, use the orthonormalization $\langle p|p'\rangle = \delta[p-p']$, the resolution of the identity $I = \int dx\,|x\rangle\langle x|$, and the Dirac delta representation $\delta[p] = \int dx\, e^{ipx/\hbar}/(2\pi\hbar)$.

(c) Use the state expansion

$$|\psi\rangle = I|\psi\rangle = \int dx\,|x\rangle\langle x|\psi\rangle \tag{4.118}$$

to show that the position wave functions $\psi[x] = \langle x|\psi\rangle$ are the *Fourier transforms* of the momentum wave functions $\tilde{\psi}[p] = \langle p|\psi\rangle$.

Chapter 5

Harmonic Oscillator

The harmonic oscillator is the most important model system in both classical and quantum physics.

5.1 Classical Harmonic Oscillator

Consider a simple (or ideal) harmonic oscillator, a mass m connected to a Hooke's law spring of stiffness k. If the displacement is x, then the linear restoring force is $F_x = -kx$, and the quadratic (or parabolic) potential energy function is

$$V[x] = \frac{1}{2}kx^2. \tag{5.1}$$

The equation of motion follows from Newton's second law $a_x = F_x/m$, namely

$$\ddot{x} = \partial_t^2 x = -\frac{1}{m}\partial_x V = -\frac{1}{m}V'[x] = -\frac{k}{m}x. \tag{5.2}$$

This has the well-known sinusoidal solution

$$x[t] = A\sin[\omega t + \varphi], \tag{5.3}$$

provided the angular frequency $\omega = \sqrt{k/m}$. The constants A and φ depend on the initial conditions. In phase space $\{x, p_x\}$, energy

$$E = \frac{1}{2}mv_x^2 + V[x] = \frac{1}{2m}p_x^2 + \frac{m\omega^2}{2}x^2 \tag{5.4}$$

conservation implies elliptical orbits.

Real springs, of course, aren't so simple. Stretch them too far, for example, and they break. However, almost any potential energy function is approximately parabolic near a local minimum. If the potential $V[x]$ has a minimum at x_0, expand in a Taylor series to get

$$V[x] = V[x_0] + V'[x_0]\,(x - x_0) + \frac{1}{2}V''[x_0](x - x_0)^2 + \cdots. \tag{5.5}$$

Since $V'[x_0] = 0$, near x_0

$$V[x] - V[x_0] \sim \frac{1}{2} V''[x_0](x - x_0)^2 \tag{5.6}$$

or

$$\delta V \sim \frac{1}{2} k (\delta x)^2, \tag{5.7}$$

where $k = V''[x_0]$. Thus, the simple harmonic oscillator is a canonical system of widespread importance.

5.2 Commutator Solution

Quantum mechanically, the Eq. 5.4 harmonic oscillator oscillator implies the Hamiltonian operator

$$H = \frac{1}{2m} P^2 + \frac{m\omega^2}{2} Q^2, \tag{5.8}$$

where the energy spectrum of H follows algebraically from the Table 4.3 commutation relation

$$[Q, P] = i\hbar I, \tag{5.9}$$

and the hermeticity of the position and momentum operators.

5.2.1 Dimensionless Variables

An oscillator of energy

$$\frac{1}{2}\hbar\omega = \frac{1}{2m} p_x^2 + \frac{m\omega^2}{2} x^2 = \frac{1}{2m} p_0^2 + 0 = 0 + \frac{m\omega^2}{2} x_0^2 \tag{5.10}$$

defines a maximum position $x_0 = \sqrt{\hbar/m\omega}$ and momentum $p_0 = \sqrt{m\hbar\omega}$, which define *dimensionless operators*

$$q = \frac{Q}{x_0} = \sqrt{\frac{m\omega}{\hbar}} Q, \tag{5.11a}$$

$$p = \frac{P}{p_0} = \sqrt{\frac{1}{m\hbar\omega}} P, \tag{5.11b}$$

so that

$$[q, p] = \left[\sqrt{\frac{m\omega}{\hbar}} Q, \sqrt{\frac{1}{m\hbar\omega}} P \right] = \frac{1}{\hbar} [Q, P] = i, \tag{5.12}$$

where the identity operator I is implicit in the final step, as is conventional. The Eq. 5.8 Hamiltonian becomes

$$H = \frac{1}{2m} \left(m\hbar\omega\, p^2 \right) + \frac{m\omega^2}{2} \left(\frac{\hbar}{m\omega} q^2 \right) = \frac{1}{2}\hbar\omega \left(p^2 + q^2 \right). \tag{5.13}$$

5.2.2 Creation & Annihilation Operators

Introduce *creation* and *annihilation* operators

$$a = \frac{q + ip}{\sqrt{2}}, \tag{5.14a}$$

$$a^\dagger = \frac{q - ip}{\sqrt{2}}, \tag{5.14b}$$

such that

$$q = \frac{a + a^\dagger}{\sqrt{2}}, \tag{5.15a}$$

$$p = \frac{a - a^\dagger}{i\sqrt{2}}, \tag{5.15b}$$

and

$$[a, a^\dagger] = \frac{1}{2}\Big([q, q] - i[q, p] + i[p, q] + [p, p]\Big) = -i[q, p] = 1. \tag{5.16}$$

Substitute the Eq. 5.15 dimensionless operators into the Eq. 5.119 Hamiltonian to "factorize" it into

$$\begin{aligned} H &= \frac{1}{2}\hbar\omega\left(\frac{-(a - a^\dagger)^2 + (a + a^\dagger)^2}{2}\right) \\ &= \frac{1}{2}\hbar\omega\left(aa^\dagger + a^\dagger a\right) \\ &= \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \\ &= \hbar\omega\left(N + \frac{1}{2}\right), \end{aligned} \tag{5.17}$$

where the hermitian *number* operator

$$N = a^\dagger a = (a^\dagger a)^\dagger = N^\dagger \tag{5.18}$$

obeys

$$[N, a] = [a^\dagger a, a] = a^\dagger[a, a] + [a^\dagger, a]a = -a, \tag{5.19a}$$

$$[N, a^\dagger] = [a^\dagger a, a^\dagger] = a^\dagger[a, a^\dagger] + [a^\dagger, a^\dagger]a = +a^\dagger. \tag{5.19b}$$

5.2.3 Number Operator Spectrum

Let $|\lambda\rangle$ be an eigenstate of the number operator N with eigenvalue λ so that

$$N|\lambda\rangle = \lambda|\lambda\rangle. \tag{5.20}$$

First "annihilate" or "lower" an eigenstate to $a|\lambda\rangle$ and apply the number operator

$$Na|\lambda\rangle = (aN + [N,a])|\lambda\rangle = (aN - a)|\lambda\rangle = (a\lambda - a)|\lambda\rangle = (\lambda - 1)a|\lambda\rangle \tag{5.21}$$

to show that

$$a|\lambda\rangle \propto |\lambda - 1\rangle \tag{5.22}$$

is an eigenstate with eigenvalue $\lambda - 1$,

$$N|\lambda - 1\rangle = (\lambda - 1)|\lambda - 1\rangle. \tag{5.23}$$

Similarly, show that

$$a^2|\lambda - 2\rangle \propto |\lambda - 2\rangle \tag{5.24}$$

is an eigenstate with eigenvalue $\lambda - 2$,

$$N|\lambda - 2\rangle = (\lambda - 2)|\lambda - 2\rangle. \tag{5.25}$$

Continue to create a downward "ladder" of eigenstates and eigenvalues. The ladder must have a bottom rung, because if $|\mu\rangle = a|\lambda\rangle$, then

$$0 \leq \langle\mu|\mu\rangle = \langle\lambda|a^\dagger a|\lambda\rangle = \langle\lambda|N|\lambda\rangle = \lambda\langle\lambda|\lambda\rangle = \lambda \tag{5.26}$$

must be nonnegative. Let $|\psi\rangle = |0\rangle$ be the *vacuum state* such that

$$a|0\rangle = 0, \tag{5.27}$$

so that further annihilations will produce no more eigenstates. Normalize the annihilation operator such that

$$a|n\rangle = c_n|n-1\rangle, \tag{5.28}$$

where

$$n = \langle n|N|n\rangle = \langle n|a^\dagger a|n\rangle = \langle n-1|c_n^* c_n|n-1\rangle = |c_n|^2. \tag{5.29}$$

Choose a real and positive normalization $c_n = \sqrt{n}$ so that

$$a|n\rangle = \sqrt{n}|n-1\rangle. \tag{5.30}$$

Next "create" or "raise" an eigenstate to $a^\dagger|\lambda\rangle$ and apply the number operator

$$Na^\dagger|\lambda\rangle = (a^\dagger N + a^\dagger)|\lambda\rangle = (a^\dagger\lambda + a^\dagger)|\lambda\rangle = (\lambda + 1)a^\dagger|\lambda\rangle \tag{5.31}$$

to show that

$$a^\dagger|\lambda\rangle \propto |\lambda + 1\rangle \tag{5.32}$$

is an eigenstate with eigenvalue $\lambda + 1$,

$$N|\lambda + 1\rangle = (\lambda + 1)|\lambda + 1\rangle. \tag{5.33}$$

Similarly, show that

$$(a^\dagger)^2|\lambda + 2\rangle \propto |\lambda + 2\rangle \tag{5.34}$$

is an eigenstate with eigenvalue $\lambda + 2$,

$$N|\lambda + 2\rangle = (\lambda + 2)|\lambda + 2\rangle. \tag{5.35}$$

Continue to create an upward "ladder" of eigenstates and eigenvalues. The ladder does not have a top rung. Normalize the creation operator by

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \tag{5.36}$$

5.2.4 Energy Spectrum

Thus, the orthonormal eigenstates of the number operator satisfy

$$N|n\rangle = n|n\rangle \tag{5.37}$$

for nonnegative integers $n = 0, 1, 2, \ldots$, and by Eq. 5.17, the orthonormal eigenstates of the Hamiltonian operator satisfy

$$H|E_n\rangle = E_n|E_n\rangle, \tag{5.38}$$

where

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{5.39}$$

The ground state or *zero-point energy* $E_0 = \hbar\omega/2$ is nonzero due to the Heisenberg uncertainty principle. If it were zero, the oscillator's position and momentum would be both be exactly zero, but if one of the two is exact, the other must be indeterminate. The zero-point energy of the quantum vacuum *may* be related to the Dark Energy (or Clear Tension) that seems to be accelerating the expansion of the universe.

The regular energy spacing $\varDelta E = E_{n+1} - E_n = \hbar\omega$ makes possible the photon model of light. Transitions between adjacent energy levels are accompanied by the emission or absorption of photons of energy $\hbar\omega$, corresponding to classical light of temporal frequency ω.

5.2.5 Wave Functions

The harmonic oscillator wave functions

$$\psi_n[x] = \langle x|n\rangle \tag{5.40}$$

are the projections of the eigenstates $|n\rangle$ in the position basis. For example, find the ground state wave function by projecting the vacuum state annihilation

$$0 = a|0\rangle = \frac{q + ip}{\sqrt{2}}|0\rangle = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}Q + i\sqrt{\frac{1}{m\hbar\omega}}P\right)|0\rangle \tag{5.41}$$

on the position basis

$$0 = \sqrt{\frac{m\omega}{\hbar}}\langle x|Q|0\rangle + i\sqrt{\frac{1}{m\hbar\omega}}\langle x|P|0\rangle = \sqrt{\frac{m\omega}{\hbar}}x\,\psi_0[x] + i\sqrt{\frac{1}{m\hbar\omega}}\left(-i\hbar\partial_x\psi_0[x]\right) \tag{5.42}$$

using the Eq. 4.107 and Eq. 4.102 representations for the position and momentum operators in the position basis to get the differential equation

$$-\frac{m\omega}{\hbar}x\psi_0 = \frac{d\psi}{dx}. \tag{5.43}$$

Separate variables

$$-\frac{m\omega}{\hbar}x dx = \frac{d\psi}{\psi_0} \tag{5.44}$$

and integrate

$$-\frac{m\omega}{\hbar}\frac{x^2}{2} = \log\psi_0 - \log N_0 \tag{5.45}$$

to find the gaussian ground state wave function

$$\psi_0[x] = N_0 e^{-m\omega x^2/2\hbar} = N_0 e^{-\frac{1}{2}(x/x_0)^2}, \tag{5.46}$$

where N_0 is a normalization constant.

5.3 Differential Equation Solution

An alternate approach to finding the spectrum of the quantum harmonic oscillator is to solve the eigenvalue problem

$$H|E\rangle = E|E\rangle \tag{5.47}$$

for the Eq. 5.8 Hamiltonian in the position basis

$$\langle x|H|E\rangle = E\langle x|E\rangle, \tag{5.48}$$

which implies the differential equation

$$\frac{1}{2m}(-i\hbar\partial_x)^2\psi_E[x] + \frac{m\omega^2}{2}x^2\psi_E[x] = E\psi_E[x] \tag{5.49}$$

or

$$-\frac{\hbar^2}{2m}\psi'' + \frac{m\omega^2}{2}\psi = E\psi, \tag{5.50}$$

where $\psi = \psi_E[x] \in \mathcal{R}$ is real for simplicity, subject to the normalization constraint

$$1 = \langle E|E\rangle = \int dx\,\langle E|x\rangle\langle E|x\rangle = \int_{-\infty}^{\infty} dx\,\psi_E[x]^*\psi_E[x] = \int_{-\infty}^{\infty} dx\,\psi^2. \tag{5.51}$$

This famous problem is nontrivial.

5.3.1 Dimensionless Variables

Again introduce dimensionless variables. For the position scale, let x_0 be the classical turning point for a harmonic oscillator with energy $E_0 = \hbar\omega/2$. Thus

$$\frac{1}{2}\hbar\omega = E_0 = \frac{1}{2}mv^2 + \frac{1}{2}kx^2 = 0 + \frac{1}{2}kx_0^2, \tag{5.52}$$

which implies

$$x_0 = \sqrt{\frac{\hbar\omega}{k}} = \sqrt{\frac{\hbar}{m\omega}}. \tag{5.53}$$

Use this scale to define a dimensionless position

$$\xi = \frac{x}{x_0} \tag{5.54}$$

and a dimensionless eigenfunction

$$\varphi[\xi] = \sqrt{x_0}\,\psi[x]. \tag{5.55}$$

Then the derivatives transform like

$$\psi' = \frac{d\psi}{dx} = \frac{1}{\sqrt{x_0}}\frac{d\varphi}{dx} = \frac{1}{\sqrt{x_0}}\frac{d\xi}{dx}\frac{d\varphi}{d\xi} = \frac{1}{{x_0}^{3/2}}\varphi' \tag{5.56}$$

and

$$\psi'' = \frac{d\psi'}{dx} = \frac{1}{{x_0}^{3/2}}\frac{d\varphi'}{dx} = \frac{1}{{x_0}^{3/2}}\frac{d\xi}{dx}\frac{d\varphi'}{d\xi} = \frac{1}{{x_0}^{5/2}}\varphi'', \tag{5.57}$$

where, as usual, the prime denotes derivative with respect to the argument (x or ξ, as appropriate). Putting this altogether, our problem transforms to solving

$$\varphi'' = \left(\xi^2 - \epsilon\right)\varphi \tag{5.58}$$

subject to the constraint

$$1 = \int_{-\infty}^{\infty} d\xi\, \varphi^2, \tag{5.59}$$

where the dimensionless energy

$$\epsilon = \frac{E}{E_0}. \tag{5.60}$$

5.3.2 Asymptotic Behavior

When ξ is large, neglect ϵ and write

$$\varphi'' \sim \xi^2\varphi, \tag{5.61}$$

which has the approximate exponential solutions

$$\varphi \sim \pm e^{\pm\frac{1}{2}\xi^2}. \tag{5.62}$$

To verify this, note that

$$\varphi' \sim \xi e^{\pm\frac{1}{2}\xi^2} \tag{5.63}$$

and

$$\varphi'' \sim \left(\pm 1 + \xi^2\right) e^{\pm\frac{1}{2}\xi^2} \sim \xi^2 \varphi. \tag{5.64}$$

Since only the decaying exponential is square normalizable, strip off the asymptotic behavior by assuming solutions of the form

$$\varphi[\xi] = h[\xi] e^{-\frac{1}{2}\xi^2}, \tag{5.65}$$

and expect the functions $h[\xi]$ to be polynomials. Then

$$\varphi' = \left(h' - \xi h\right) e^{-\frac{1}{2}\xi^2} \tag{5.66}$$

and

$$\varphi'' = \left(h'' - 2\xi h' + \left(\xi^2 - 1\right) h\right) e^{-\frac{1}{2}\xi^2}. \tag{5.67}$$

With these substitutions, the exponentials cancel, and our differential equation becomes

$$h'' - 2\xi h' + \left(\epsilon - 1\right) h = 0. \tag{5.68}$$

5.3.3 Power Series Solution

Write the solution as a power series

$$h[\xi] = a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \cdots = \sum_{m=0}^{\infty} a_m \xi^m, \tag{5.69}$$

and its first derivative

$$h'[\xi] = 0 + a_1 + 2a_2 \xi + 3a_3 \xi^2 + \cdots = \sum_{m=0}^{\infty} m a_m \xi^{m-1}, \tag{5.70}$$

and its second derivative

$$h''[\xi] = 0 + 0 + 2a_2 + 3 \cdot 2a_3 \xi + \cdots = \sum_{m=0}^{\infty} m\left(m-1\right) a_m \xi^{m-2}. \tag{5.71}$$

Substituting these power series into Eq. 5.68 gives

$$\sum_{m=0}^{\infty} m\left(m-1\right) a_m \xi^{m-2} - 2\xi \sum_{m=0}^{\infty} m a_m \xi^{m-1} + \left(\epsilon - 1\right) \sum_{m=0}^{\infty} a_m \xi^m = 0. \tag{5.72}$$

By shifting the dummy index $m \to m+2$ in first summation, consolidate this as

$$\sum_{m=0}^{\infty} \left(\left(m+2\right)\left(m+1\right) a_{m+2} - 2m a_m + \left(\epsilon - 2\right) a_m\right) \xi^m = 0. \tag{5.73}$$

The only way this can be true *for all* ξ is if the coefficients are all zero, which means

$$a_{m+2} = \frac{2m+1-\epsilon}{(m+1)(m+2)} a_m. \tag{5.74}$$

This *recursion relation* separately links coefficients of odd and even indices. It thereby specifies two independent solutions, corresponding to the two arbitrary constants determined by the initial conditions of our second-order differential equation. The constant a_0 specifies symmetric solutions $h[-\xi] = h[\xi]$ in even powers of ξ, while the constant a_1 specifies antisymmetric solutions $h[-\xi] = -h[\xi]$ in odd powers of ξ. This is consistent with our expectation that symmetric potentials $V[-x] = V[x]$ imply eigenfunctions of definite symmetry $\psi[-x] = \pm\psi[x]$.

5.3.4 Power Series Diverges

For large $m \gg 1$, the recursion relation simplifies to

$$a_{m+2} \sim \frac{2m}{m \cdot m} a_m = \frac{a_m}{m/2}. \tag{5.75}$$

This has the approximate solution

$$a_m \sim \frac{K}{(m/2)!}, \tag{5.76}$$

for some constant K, because it implies

$$a_{m+2} \sim \frac{K}{(m/2+1)!} = \frac{K}{(m/2+1)(m/2)!} \sim \frac{a_m}{m/2+1} \sim \frac{a_m}{m/2}. \tag{5.77}$$

However, this means

$$h[\xi] \sim \sum_{m \gg 1} \frac{K}{(m/2)!} \xi^m = K \sum_{m \gg 1} \frac{\left(\xi^2\right)^{m/2}}{(m/2)!} \sim K \sum_{l=0}^{\infty} \frac{\left(\xi^2\right)^l}{l!} = K e^{\xi^2}. \tag{5.78}$$

Thus

$$\varphi[\xi] = h[\xi] e^{-\frac{1}{2}\xi^2} \sim \tilde{K} e^{+\frac{1}{2}\xi^2}, \tag{5.79}$$

for some constant $\tilde{K}$. This divergent and unnormalizable behavior is unacceptable.

5.3.5 Truncate Series

The only way to avoid nonphysical solutions is for the infinite power series to terminate. This can happen if the numerator of the recursion relation vanishes for some $m = n < \infty$, in which case $a_{n+2} = 0$ and hence $a_{m \geq n+2} = 0$. The only way for the numerator to vanish is if the dimensionless energy ϵ is quantized according to

$$\epsilon_n = 2n + 1, \tag{5.80}$$

which implies that the dimensional energy E is quantized according to

$$E_n = \epsilon_n E_0 = (2n+1)\,\frac{\hbar\omega}{2} = \left(n + \frac{1}{2}\right)\hbar\omega, \tag{5.81}$$

for $n = 0, 1, 2, \ldots$. Thus, the physically relevant recursion relation is

$$a_{m+2} = \frac{2m + 1 - \epsilon_n}{(m+1)\,(m+2)} a_m = -\frac{2\,(n-m)}{(m+1)\,(m+2)} a_m, \tag{5.82}$$

where $m = 0, 1, 2, \ldots, n$. This defines a symmetric or antisymmetric nth order *hermite polynomial* $H_n[\xi]$.

5.3.6 Standard Form Solutions

Write the harmonic oscillator eigenfunctions in standard form as

$$\psi_n[x] = N_n H[x/x_0] e^{-\frac{1}{2}(x/x_0)^2}, \tag{5.83}$$

where x_0 is the classical turning point of Eq. 5.53 and the normalization constant

$$N_n = \frac{1}{\sqrt{x_0 2^n n! \sqrt{\pi}}} \tag{5.84}$$

is fixed by the constraint Eq. 5.51. The first few eigenfunctions are listed in Table 5.1 and graphed in Figure 5.1.

Table 5.1: First few harmonic oscillator eigenvalues and eigenfunctions.

n	E_n	$\psi_n[x]$
0	$\frac{1}{2}E_0$	$N_0 e^{-\frac{1}{2}(x/x_0)^2}$
1	$\frac{3}{2}E_0$	$N_1 2(x/x_0) e^{-\frac{1}{2}(x/x_0)^2}$
2	$\frac{5}{2}E_0$	$N_2(-2 + 4(x/x_0)^2) e^{-\frac{1}{2}(x/x_0)^2}$
3	$\frac{7}{2}E_0$	$N_3(-12(x/x_0) + 8(x/x_0)^3) e^{-\frac{1}{2}((x/x_0))^2}$

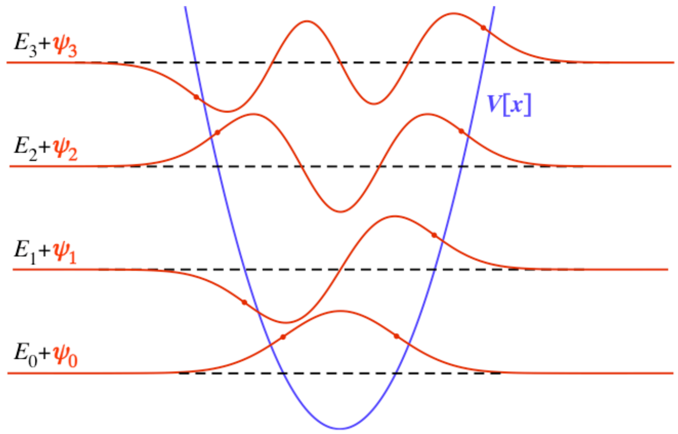


Figure 5.1: First few harmonic oscillator eigenfunctions superimposed on the corresponding energy eigenvalues of the quadratic potential. The dots denote concavity changes, the smooth joining of sinusoids and exponentials, at the classical turning points.

5.3.7 Classical Correspondence

Quantum harmonic oscillator states of small quantum number n do not have classical analogues. In fact, such eigenfunctions are very wave-like, dominated by nodes near which the probability of finding the particle is near zero. However, recover a classical correspondence by considering states of large quantum number.

For comparison, first compute the probability distribution for a classical harmonic oscillator. The sinusoidally oscillating position of Eq. 5.3,

$$x = A\sin[\omega t + \varphi], \tag{5.85}$$

implies a sinusoidally oscillating velocity

$$\dot{x} = v_x = \omega A\cos[\omega t + \varphi]. \tag{5.86}$$

Together, these imply an elliptical phase space $\{x[t], v_x[t]\}$ trajectory

$$x^2 + \left(\frac{v_x}{\omega}\right)^2 = A^2 \tag{5.87}$$

and a speed

$$|v_x| = \omega\sqrt{A^2 - x^2}. \tag{5.88}$$

Suppose the oscillator mass m spends a time dt in distance dx about position x. The probability of finding it there is inversely proportional to its speed, so

$$d\mathcal{P} = \rho_c[x]dx = Cdt = C\frac{dx}{|v_x|} = C\frac{dx}{\omega\sqrt{A^2 - x^2}}, \tag{5.89}$$

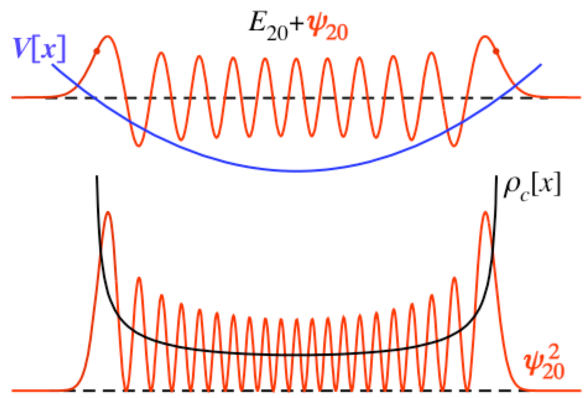


Figure 5.2: At even the modest quantum number $n = 20$, the quantum probability density corresponds well to the classical probability density.

where the normalization constant C is determined by the constraint

$$1 = \int_{-A}^{A} \rho_c[x] dx = \int_{t_0}^{t_0+T/2} C dt = C\frac{T}{2}. \tag{5.90}$$

Thus, $C = 2/T = \omega/\pi$, and the classical probability density is

$$\rho_c[x] = \frac{1}{\pi\sqrt{A^2 - x^2}}. \tag{5.91}$$

The classical turning point coordinate x_n corresponding to the energy E_n is defined by

$$(2n+1)\, E_0 = E_n = V[x_n] = E_0 \left(\frac{x_n}{x_0}\right)^2, \tag{5.92}$$

or

$$x_n = x_0\sqrt{2n+1}. \tag{5.93}$$

The quantum probability density follows the classical probability density with $A = x_n$, as in Figure 5.2, for $n = 20$.

5.4 Angular Momentum

Harmonic oscillators in higher dimensions can have nonzero angular momentum. To model such oscillators, first study the eigenstates and eigenvalues of the angular momentum operators $J_a = J_a^\dagger$, which are completely determined by the Table 4.3 commutation relations

$$[J_a, J_b] = i\hbar\, \epsilon_{abc} J_c. \tag{5.94}$$

Although the components of angular momenta don't commute with each other, they do commute with the the total angular momentum squared,

$$\begin{aligned}[J^2, J_b] &= [J_a J_a, J_b] \\ &= J_a[J_a, J_b] + [J_a, J_b]J_a \\ &= J_a \epsilon_{abc} J_c + \epsilon_{abc} J_c J_a \\ &= \epsilon_{abc} J_a J_c + \epsilon_{cba} J_a J_c \\ &= (\epsilon_{abc} + \epsilon_{cba}) J_a J_c \\ &= (\epsilon_{abc} - \epsilon_{abc}) J_a J_c \\ &= 0, \end{aligned} \tag{5.95}$$

and therefore share common eigenstates

$$J^2|s, c\rangle = \hbar^2 s|s, c\rangle, \tag{5.96a}$$

$$J_z|s, c\rangle = \hbar\ c|s, c\rangle, \tag{5.96b}$$

where the index choice $a = 3 = z$ is conventional (from its special role in cylindrical and spherical coordinates), and the factors of $\hbar$ make the squared and component quantum numbers s and c dimensionless.

The expectation of any component squared

$$\left\langle J_a^2 \right\rangle = \left\langle s, c\middle|J_a^2\middle|s, c\right\rangle = \left(\left\langle s, c\middle|J_a^\dagger\right)\left(J_a\middle|s, c\right\rangle\right) = \langle\varphi|\varphi\rangle \geq 0 \tag{5.97}$$

must be positive, and so the expectation of the total momentum squared

$$\left\langle s, c\middle|J^2\middle|s, c\right\rangle = \left\langle s, c\middle|J_x^2\middle|s, c\right\rangle + \left\langle s, c\middle|J_y^2\middle|s, c\right\rangle + \left\langle s, c\middle|J_z^2\middle|s, c\right\rangle \tag{5.98}$$

implies

$$\hbar^2 s = \left\langle J_x^2 \right\rangle + \left\langle J_y^2 \right\rangle + \hbar^2 c^2 \geq \hbar^2 c^2 \tag{5.99}$$

and

$$-\sqrt{s} \leq c \leq +\sqrt{s}. \tag{5.100}$$

As with the harmonic oscillator, define the raising and lowering operators

$$J_\pm = J_x \pm iJ_y, \tag{5.101}$$

which satisfy

$$[J_z, J_\pm] = [J_z, J_x \pm iJ_y] = [J_z, J_x] \pm i[J_z, J_y] = i\hbar J_y \pm \hbar J_x = \pm\hbar J_\pm \tag{5.102}$$

and

$$[J_+, J_-] = [J_x + iJ_y, J_x - iJ_y] = [J_x, J_x] - i[J_x, J_y] + i[J_y, J_x] + [J_y, J_y] = 2\hbar J_z. \tag{5.103}$$

First raise an eigenstate to $J_+|s, c\rangle$ and measure J_z by applying the component operator to get

$$J_z J_+|s, c\rangle = (J_+ J_z + [J_z, J_+])|s, c\rangle = (J_+ J_z + \hbar J_+)|s, c\rangle = \hbar(c + 1)J_+|s, c\rangle \tag{5.104}$$

and show that

$$J_+|s,c\rangle \propto |s,c+1\rangle \tag{5.105}$$

is an eigenstate of J_z with eigenvalue $\hbar(c+1)$. The raising operator must annihilate the state with the maximum component

$$J_+|s,c_{\max}\rangle = 0 \tag{5.106}$$

or it would create an eigenstate with eigenvalue larger than the maximum. Since

$$J_-J_+ = (J_x - iJ_y)(J_x + iJ_y) = J_x^2 + J_y^2 + i(J_xJ_y - J_yJ_x) = J^2 - J_z^2 - \hbar J_z, \tag{5.107}$$

multiply Eq. 5.106 by the lowering operator to find

$$0 = J_-J_+|s,c_{\max}\rangle = \hbar^2(s - c_{\max}^2 - c_{\max})|s,c_{\max}\rangle \tag{5.108}$$

so

$$s = c_{\max}(c_{\max}+1). \tag{5.109}$$

Next lower an eigenstate to $J_-|s,c\rangle$ and measure J_z by applying the component operator to get

$$J_zJ_-|s,c\rangle = (J_-J_z + [J_z,J_-])|s,c\rangle = (J_-J_z - \hbar J_-)|s,c\rangle = \hbar(c-1)J_-|s,c\rangle \tag{5.110}$$

and show that

$$J_-|s,c\rangle \propto |s,c-1\rangle \tag{5.111}$$

is an eigenstate of J_z with eigenvalue $\hbar(c-1)$. The lower operator must annihilate the state with the minimum component

$$J_-|s,c_{\min}\rangle = 0 \tag{5.112}$$

or it would create an eigenstate with eigenvalue smaller than the minimum. Since

$$J_+J_- = (J_x + iJ_y)(J_x - iJ_y) = J_x^2 + J_y^2 - i(J_xJ_y - J_yJ_x) = J^2 - J_z^2 + \hbar J_z, \tag{5.113}$$

multiply Eq. 5.112 by the raising operator to find

$$0 = J_+J_-|s,c_{\min}\rangle = \hbar^2(s - c_{\min}^2 + c_{\min})|s,c_{\min}\rangle \tag{5.114}$$

so

$$s = -c_{\min}(-c_{\min}+1). \tag{5.115}$$

Equations 5.109 & 5.115 imply $c_{\max} = -c_{\min} \equiv j$ so that $s = j(j+1)$. Since the component quantum numbers c differ by integers, $c_{\max} - c_{\min} = 2j$ is an integer, and j is a "half integer". Conventionally label the common eigenstates of J^2 and J_z by quantum numbers j and $m = c$ so that

$$J^2|j,m\rangle = \hbar^2 j(j+1)|j,m\rangle, \tag{5.116a}$$

$$J_z|j,m\rangle = \hbar\, m|j,m\rangle, \tag{5.116b}$$

where each angular momentum *squared* quantum number $j = 0, 1/2, 1, 3/2, 2, \ldots$ corresponds to $2j+1$ values of angular momentum *component* quantum number $m = -j, -j+1, \ldots, j-1, j$, as in Fig. 5.3. In nature, *fermions* (like electrons) realize the half integer spin angular momentum and *bosons* (like photons) realize the integer spin angular momentum.

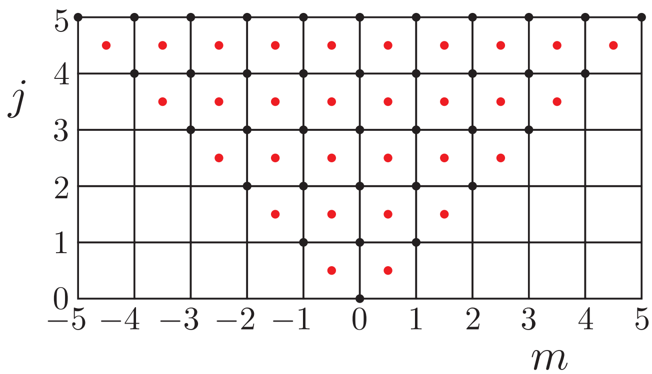


Figure 5.3: Angular momentum quantum numbers for fermions (red dots) and bosons (black dots).

5.5 Two-Dimensional Harmonic Oscillator

5.5.1 Classical Case

An isotropic harmonic oscillator in the two-dimensional xy-plane has energy

$$E = \frac{1}{2m}p_x^2 + \frac{1}{2m}p_x^2 + \frac{m\omega^2}{2}(x^2 + y^2), \tag{5.117}$$

and angular momentum

$$\vec{L} = \vec{r} \times \vec{p} = \hat{z}(xp_y - yp_x). \tag{5.118}$$

5.5.2 Eigenstates of Energy

Quantum mechanically, the Eq. 5.117 harmonic oscillator oscillator implies the Hamiltonian operator

$$H = \frac{1}{2m}P_x^2 + \frac{1}{2m}P_y^2 + \frac{m\omega^2}{2}(X^2 + Y^2), \tag{5.119}$$

where the energy spectrum of H follows algebraically from the Table 4.3 commutation relations

$$[X, P_x] = i\hbar, \tag{5.120a}$$
$$[Y, P_y] = i\hbar, \tag{5.120b}$$

with all others vanishing, and the hermeticity of the position and momentum operators.

Mirroring the solution of the one-dimensional oscillator, introduce the dimensionless position and momentum operators

$$x = \frac{X}{x_0} = \sqrt{\frac{m\omega}{\hbar}}X, \tag{5.121a}$$

$$y = \frac{Y}{x_0} = \sqrt{\frac{m\omega}{\hbar}}Y, \tag{5.121b}$$

$$p_x = \frac{P_x}{p_0} = \sqrt{\frac{1}{m\hbar\omega}}P_x, \tag{5.121c}$$

$$p_y = \frac{P_y}{p_0} = \sqrt{\frac{1}{m\hbar\omega}}P_y, \tag{5.121d}$$

and the annihilation or creation operators

$$a_x = \frac{x + ip_x}{\sqrt{2}}, \tag{5.122a}$$

$$a_y = \frac{y + ip_y}{\sqrt{2}}, \tag{5.122b}$$

$$a_x^\dagger = \frac{x - ip_x}{\sqrt{2}}, \tag{5.122c}$$

$$a_y^\dagger = \frac{y - ip_y}{\sqrt{2}}, \tag{5.122d}$$

such that

$$x = \frac{a_x + a_x^\dagger}{\sqrt{2}}, \tag{5.123a}$$

$$y = \frac{a_y + a_y^\dagger}{\sqrt{2}}, \tag{5.123b}$$

$$p_x = \frac{a_x - a_x^\dagger}{i\sqrt{2}}, \tag{5.123c}$$

$$p_y = \frac{a_y - a_y^\dagger}{i\sqrt{2}}, \tag{5.123d}$$

and

$$[a_x, a_x^\dagger] = 1 = [a_y, a_y^\dagger], \tag{5.124}$$

with all others vanishing. The Hamiltonian "factorizes" into

$$\begin{aligned} H &= \hbar\omega\left(a_x^\dagger a_x + \frac{1}{2}\right) + \hbar\omega\left(a_y^\dagger a_y + \frac{1}{2}\right) \\ &= \hbar\omega\left(N_x + \frac{1}{2}\right) + \hbar\omega\left(N_y + \frac{1}{2}\right), \\ &= \hbar\omega\left(N_x + N_y + 1\right). \end{aligned} \tag{5.125}$$

Since $[N_x, N_y] = 0$, there are simultaneous eigenstates $|n_x, n_y\rangle$ that can be lowered

$$a_x|n_x, n_y\rangle = \sqrt{n_x}|n_x - 1, n_y\rangle, \tag{5.126a}$$
$$a_y|n_x, n_y\rangle = \sqrt{n_y}|n_x, n_y - 1\rangle, \tag{5.126b}$$

and raised

$$a_x^\dagger|n_x, n_y\rangle = \sqrt{n_x + 1}|n_x + 1, n_y\rangle, \tag{5.127a}$$
$$a_y^\dagger|n_x, n_y\rangle = \sqrt{n_y + 1}|n_x, n_y + 1\rangle. \tag{5.127b}$$

The orthonormal eigenstates of the number operators satisfy

$$N_x|n_x, n_y\rangle = n_x|n_x, n_y\rangle, \tag{5.128a}$$
$$N_y|n_x, n_y\rangle = n_y|n_x, n_y\rangle, \tag{5.128b}$$

and the orthonormal eigenstates of the Hamiltonian operator satisfy

$$H|n_x, n_y\rangle = (n_x + n_y + 1)\hbar\omega|n_x, n_y\rangle, \tag{5.129}$$

or

$$H|E_{\vec{n}}\rangle = E_{\vec{n}}|E_{\vec{n}}\rangle, \tag{5.130}$$

where

$$E_{\vec{n}} = (n + 1)\hbar\omega, \tag{5.131}$$

and $n = n_x + n_y$. Because the eigenstates $|3, 2\rangle$ and $|2, 3\rangle$ correspond to the same energy of $6\hbar\omega$, the states are two-fold *degenerate*.

5.5.3 Eigenstates of Energy & Angular Momentum

Using Eqs. 5.121 & 5.123, the angular momentum operator

$$L_z = XP_y - YP_x = i\hbar(a_x a_y^\dagger - a_x^\dagger a_y) = L_z^\dagger, \tag{5.132}$$

as in Problem 5. Adding the relations

$$[a_x a_y^\dagger - a_x^\dagger a_y,\, a_x^\dagger a_x] = +a_x a_y^\dagger + a_x^\dagger a_y, \tag{5.133a}$$
$$[a_x a_y^\dagger - a_x^\dagger a_y,\, a_y^\dagger a_y] = -a_x a_y^\dagger - a_x^\dagger a_y, \tag{5.133b}$$

implies

$$[L_z, H] = 0, \tag{5.134}$$

as in Problem 6, so the angular momentum and Hamiltonian operators will have common eigenstates. Obtain these by defining new raising and lower operators

$$a_+ = \frac{a_x + ia_y}{\sqrt{2}}, \tag{5.135a}$$

$$a_- = \frac{a_x - ia_y}{\sqrt{2}}, \tag{5.135b}$$

such that

$$a_x = \frac{a_+ + a_-}{\sqrt{2}}, \tag{5.136a}$$

$$a_y = \frac{a_+ - a_-}{i\sqrt{2}}, \tag{5.136b}$$

and

$$[a_+, a_+^\dagger] = 1 = [a_-, a_-^\dagger], \tag{5.137}$$

with all others vanishing.

The Hamiltonian operator

$$\begin{aligned}\frac{H}{\hbar\omega} &= a_x^\dagger a_x + a_y^\dagger a_y + 1 \\ &= \frac{(a_+^\dagger + a_-^\dagger)(a_+ + a_-)}{2} + \frac{(a_+^\dagger - a_-^\dagger)(a_+ - a_-)}{2} + 1 \\ &= a_+^\dagger a_+ + a_-^\dagger a_- + 1 \\ &= N_+ + N_- + 1,\end{aligned} \tag{5.138}$$

and the angular momentum operator

$$\begin{aligned}\frac{L_z}{\hbar} &= i a_x a_y^\dagger - i a_x^\dagger a_y \\ &= i a_y^\dagger a_x - i a_x^\dagger a_y \\ &= -\frac{(a_+^\dagger - a_-^\dagger)(a_+ + a_-)}{2} - \frac{(a_+^\dagger + a_-^\dagger)(a_- - a_-)}{2} \\ &= -a_+^\dagger a_+ + a_-^\dagger a_- \\ &= N_- - N_+.\end{aligned} \tag{5.139}$$

The lowering operators satisfy

$$a_+|n_+, n_-\rangle = \sqrt{n_+}|n_+ - 1, n_-\rangle, \tag{5.140a}$$

$$a_-|n_+, n_-\rangle = \sqrt{n_-}|n_+, n_- - 1\rangle, \tag{5.140b}$$

and the raising operators satisfy

$$a_+^\dagger|n_+, n_-\rangle = \sqrt{n_+ + 1}|n_+ + 1, n_-\rangle, \tag{5.141a}$$

$$a_-^\dagger|n_+, n_-\rangle = \sqrt{n_- + 1}|n_+, n_- + 1\rangle, \tag{5.141b}$$

The orthonormal eigenstates of the number operators satisfy

$$N_+|n_+, n_-\rangle = n_+|n_+, n_-\rangle, \tag{5.142a}$$

$$N_-|n_+, n_-\rangle = n_-|n_+, n_-\rangle, \tag{5.142b}$$

and the orthonormal eigenstates of the Hamiltonian and angular momentum operators satisfy

$$H|n_+, n_-\rangle = (n_+ + n_- + 1)\,\hbar\omega\,|n_+, n_-\rangle, \tag{5.143a}$$

$$L_z|n_+, n_-\rangle = (n_- - n_+)\,\hbar\,|n_+, n_-\rangle. \tag{5.143b}$$

In terms of the sum and difference quantum numbers

$$n = n_+ + n_-, \tag{5.144a}$$

$$m = n_- - n_+, \tag{5.144b}$$

the dynamic operators are

$$H|n, m\rangle = (n + 1)\,\hbar\omega\,|n, m\rangle, \tag{5.145a}$$

$$L_z|n, m\rangle = m\,\hbar\,|n, m\rangle, \tag{5.145b}$$

where $n = 0, 1, 2, \ldots$ and $m = -n, -n+2, \ldots, n-2, n$. Thus for each energy, there are $n + 1$ angular momentum states, with equal numbers of positive and negative momenta.

Problems

1. Justify the Eq. 5.36 creation operator normalization.
2. Sketch the five top-left rows and columns of the infinite square matrix representations for the annihilation a, creation $a^\dagger$, and number N operators.
3. Find the constant N_0 in the Eq. 5.46 ground state wave function by enforcing Eq. 5.51 normalization.
4. Generalize the technique of Section 5.2.5 to find the harmonic oscillator first excited state position wave function $\psi_1[x] = \langle x|1\rangle$.
5. Derive the Eq. 5.132 angular momentum operator expression, and show that it is hermitian.
6. Derive the Eq. 5.133 identities and use them to show that the isotropic oscillator's Hamiltonian and angular momentum operators commute.

Chapter 6

Hydrogen Atom

The hydrogen atom is the exactly solvable model that unlocked the quantum world and underlies chemistry.

6.1 Classical Kepler Problem

The hydrogen atom problem is the quantum Kepler problem. The classical Kepler problem consist of a reduced mass article bound to an inverse distance potential

$$V[r] = -\frac{\kappa}{r}, \tag{6.1}$$

where $\kappa = GMm$ and $1/\mu = 1/m + 1/M$. Associated with the 3 degrees of freedom of the particle are $2 * 3 - 1 = 5$ constants of the motion (and a 6th related to the arbitrary origin of time). They are the total energy

$$E = \frac{p^2}{2\mu} - \frac{\kappa}{r}, \tag{6.2}$$

the angular momentum

$$\vec{L} = \vec{r} \times \vec{p}, \tag{6.3}$$

and the eccentricity (or Laplace-Runge-Lenz vector)

$$\vec{e} = \hat{r} + \frac{\vec{L} \times \vec{p}}{\mu\kappa}, \tag{6.4}$$

subject to the constraints

$$\vec{e} \cdot \vec{L} = 0 \tag{6.5}$$

and

$$e^2 = 1 + \frac{2EL^2}{\mu\kappa^2}, \tag{6.6}$$

giving $1 + 3 + 3 - 1 - 1 = 5$ constants of the motion. The last constant of the motion, the eccentricity vector $\vec{e}$, ensures that all bound orbits are closed, which is only true for the harmonic oscillator and hydrogen atom potential energies. Solve Eq. 6.6 to find the energy

$$E = -\mu\kappa^2 \frac{1-e^2}{2L^2} < 0. \tag{6.7}$$

6.2 Quantum Kepler Problem

In generalizing the classical Kepler problem to the quantum Kepler problem, the position and momentum variables become hermitian operators

$$\vec{r} = \{x, y, z\} = \{r_1, r_2, r_3\} = \{Q_1, Q_2, Q_3\}, \tag{6.8a}$$
$$\vec{p} = \{p_x, p_y, p_z\} = \{p_1, p_2, p_3\} = \{P_1, P_2, P_3\}, \tag{6.8b}$$

satisfying the Table 4.3 commutation relations. In the present notation, these imply the additional Table 6.1 commutation relations.

Table 6.1: Kepler Problem 2 commutators, where where the commutator of two vectors implicitly utilizes the scalar product, $[\vec{u}, \vec{v}] \equiv \vec{u}\cdot\vec{v} - \vec{v}\cdot\vec{u}$.

$\left[p^2,\ \vec{r}\right] = -2i\hbar\,\vec{p}$	$\left[\vec{r}\cdot\vec{p},\ \vec{r}\right] = -i\hbar\,\vec{r}$
$[\vec{p},\ 1/r] = i\hbar\,\vec{r}/r^3$	$[\vec{r}\cdot\vec{p},\ \vec{p}] = i\hbar\,\vec{p}$
$\left[p^2,\ 1/r\right] = 2i\hbar\,\vec{r}\cdot\vec{p}/r^3$	$\left[\vec{r}\cdot\vec{p},\ p^2\right] = 2i\hbar\,p^2$
$\left[\vec{p},\ 1/r^3\right] = 3i\hbar\,\vec{r}/r^5$	$[\vec{r}\cdot\vec{p},\ 1/r] = i\hbar/r$
$[\vec{p},\ \vec{r}] = -3i\hbar$	$\left[\vec{r}\cdot\vec{p},\ 1/r^3\right] = 3i\hbar/r^3$

6.2.1 Angular Momentum

To remove the ambiguity associated with the noncommutativity of the position and momentum operators, symmetrize the expression for angular momentum

$$\vec{L} = \frac{\vec{r}\times\vec{p} - \vec{p}\times\vec{r}}{2} = \frac{\vec{r}\times\vec{p} + \vec{r}\times\vec{p}}{2} = \vec{r}\times\vec{p} = \vec{L}^\dagger, \tag{6.9}$$

as the different components of position and linear momentum commute (for example, $[r_1, p_2] = [x, p_y] = 0$). The angular momentum squared

$$
\begin{aligned}
L^2 &= \vec{L} \cdot \vec{L} = L_a L_a \\
&= \epsilon_{ajk} r_j p_k \, \epsilon_{amn} r_m p_n \\
&= \epsilon_{ajk} \epsilon_{amn} r_j p_k r_m p_n \\
&= (\delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}) r_j p_k r_m p_n \\
&= r_j p_k r_j p_k - r_j p_k r_k p_j \\
&= r_j (r_j p_k + [p_k, r_j]) p_k - r_j p_k (p_j r_k + [r_k, p_j]) \\
&= r_j r_j p_k p_k - r_j i\hbar\, \delta_{kj} p_k - r_j p_k p_j r_k - r_j p_k i\hbar\, \delta_{kj} \\
&= r_j r_j p_k p_k - i\hbar\, r_j p_j - r_j p_k p_j r_k - i\hbar\, r_j p_j \\
&= r_j r_j p_k p_k - i\hbar\, r_j p_j - r_j p_j p_k r_k - i\hbar\, r_j p_j \\
&= r_j r_j p_k p_k - i\hbar\, r_j p_j - r_j p_j (r_k p_k + [p_k, r_k]) - i\hbar\, r_j p_j \\
&= r_j r_j p_k p_k - i\hbar\, r_j p_j - r_j p_j (r_k p_k - i\hbar\, \delta_{kk}) - i\hbar\, r_j p_j \\
&= r_j r_j p_k p_k - i\hbar\, r_j p_j - r_j p_j r_k p_k + 3i\hbar\, r_j p_j - i\hbar\, r_j p_j \\
&= r^2 p^2 - (\vec{r} \cdot \vec{p})^2 + i\hbar (\vec{r} \cdot \vec{p}),
\end{aligned}
\tag{6.10}
$$

as $\delta_{kk} = 1 + 1 + 1 = 3$ unless k is a fixed index.

6.2.2 Eccentricity

Symmetrize the expression for eccentricity

$$
\vec{e} = \hat{r} + \frac{\vec{L} \times \vec{p} - \vec{p} \times \vec{L}}{2\mu\kappa} = \hat{r} + \frac{\vec{L} \times \vec{p}}{\mu\kappa} - i\hbar \, \frac{\vec{p}}{\mu\kappa} = \vec{e}^{\,\dagger}, \tag{6.11}
$$

as the different components of position and angular momentum do *not* commute. However, Planck's constant is macroscopically small, and the limit $\hbar \to 0$ recovers the classical expression.

To derive the Eq. 6.11 eccentricity, write

$$
\mu\kappa \, \vec{e} = \mu\kappa \, \hat{r} + \vec{C}, \tag{6.12}
$$

where the symmetrized cross product

$$
\vec{C} = \frac{\vec{L} \times \vec{p} - \vec{p} \times \vec{L}}{2}. \tag{6.13}
$$

In components

$$
\begin{aligned}
2C_a &= \epsilon_{ajk}L_j p_k - \epsilon_{ajk}p_j L_k \\
&= \epsilon_{ajk}\epsilon_{jmn}r_m p_n p_k - \epsilon_{ajk}p_j \epsilon_{kmn}r_m p_n \\
&= -\epsilon_{ajk}\epsilon_{kmn}(r_m p_n p_j + p_j r_m p_n) \\
&= -(\delta_{am}\delta_{jn} - \delta_{an}\delta_{jm})(r_m p_n p_j + p_j r_m p_n) \\
&= -r_a p_j p_j + r_j p_a p_j - p_j r_a p_j + p_j r_j p_a \\
&= -r_a p_j p_j + r_j p_a p_j - (r_a p_j - i\hbar\,\delta_{ja})p_j + (r_j p_j - i\hbar\,\delta_{jj})p_a \\
&= -r_a p_j p_j + r_j p_a p_j - r_a p_j p_j + i\hbar\,p_a + r_j p_j p_a - 3i\hbar\,p_a \\
&= -2r_a p_j p_j + 2r_j p_j p_a - 2i\hbar\,p_a,
\end{aligned} \tag{6.14}
$$

so two forms of the cross product are

$$
\vec{C} = -\vec{r}\,p^2 + (\vec{r}\cdot\vec{p})\vec{p} - i\hbar\,\vec{p} = (\vec{r}\times\vec{p})\times\vec{p} - i\hbar\,\vec{p} = \vec{L}\times\vec{p} - i\hbar\,\vec{p}, \tag{6.15a}
$$

$$
\vec{C} = -\vec{r}\,p^2 + \vec{p}(\vec{r}\cdot\vec{p}), \tag{6.15b}
$$

where the second form is courtesy of Table 6.1. Thus, two forms of the eccentricity are

$$
\mu\kappa\,\vec{e} = \mu\kappa\,\hat{r} + \vec{L}\times\vec{p} - i\hbar\,\vec{p}, \tag{6.16a}
$$

$$
\mu\kappa\,\vec{e} = \vec{p}(\vec{r}\cdot\vec{p}) - \vec{r}\left(p^2 - \frac{\mu\kappa}{r}\right). \tag{6.16b}
$$

If $\phi = \vec{r}\cdot\vec{p}$ and $\theta = p^2 - \mu\kappa/r$, then the eccentricity squared

$$
\begin{aligned}
(\mu\kappa\,e)^2 &= \mu\kappa\,\vec{e}\cdot\mu\kappa\,\vec{e} \\
&= (\vec{p}\phi - \vec{r}\theta)\cdot(\vec{p}\phi - \vec{r}\theta) \\
&= \vec{p}\phi\cdot\vec{p}\phi - \vec{p}\phi\cdot\vec{r}\vec{\theta} - \vec{r}\theta\cdot\vec{p}\phi + \vec{r}\theta\cdot\vec{r}\phi.
\end{aligned} \tag{6.17}
$$

The Table 6.1 commutators imply

$$
\begin{aligned}
\vec{p}\phi\cdot\vec{p}\phi &= p_n\phi\,p_n\phi \\
&= p_n(p_n\phi + i\hbar\,p_n)\phi \\
&= p_n p_n\phi^2 + i\hbar\,p_n p_n\phi \\
&= p^2\phi^2 + i\hbar\,p^2
\end{aligned} \tag{6.18}
$$

and similarly

$$
-\vec{p}\phi\cdot\vec{r}\vec{\theta} = -p^2\phi^2 - \hbar^2 p^2 + \frac{\mu\kappa}{r}\phi^2 - 2i\hbar\frac{\mu\kappa}{r}\phi \tag{6.19}
$$

and

$$
-\vec{r}\theta\cdot\vec{p}\phi = -p^2\phi^2 + \frac{\mu\kappa}{r}\phi^2 - 2i\hbar\,p^2\phi \tag{6.20}
$$

and

$$+\vec{r}\theta\cdot\vec{r}\phi = +p^2r^2p^2 + 2\hbar^2p^2 - 2\mu\kappa\, rp^2 + (\mu\kappa)^2 - 2\hbar^2\frac{\mu\kappa}{r} + 2i\hbar\, p^2. \tag{6.21}$$

Hence, the eccentricity squared

$$\begin{aligned}
(\mu\kappa\, e)^2 &= +p^2\phi^2 + i\hbar\, p^2\phi \\
&\quad - p^2\phi^2 - \hbar^2p^2 + \frac{\mu\kappa}{r}\phi^2 - 2i\hbar\frac{\mu\kappa}{r}\phi \\
&\quad - p^2\phi^2 + \frac{\mu\kappa}{r}\phi^2 - 2i\hbar\, p^2\phi \\
&\quad + p^2r^2p^2 + 2\hbar^2p^2 - 2\mu\kappa\, rp^2 + (\mu\kappa)^2 - 2\hbar^2\frac{\mu\kappa}{r} + 2i\hbar\, p^2\phi \\
&= (\mu\kappa)^2 + p^2r^2p^2 - p^2\phi^2 + i\hbar\, p^2\phi - 2\mu\kappa\, rp^2 + 2\frac{\mu\kappa}{r}\phi^2 - 2i\hbar\frac{\mu\kappa}{r}\phi + \hbar^2p^2 - 2\hbar^2\frac{\mu\kappa}{r} \\
&= (\mu\kappa)^2 + p^2\left(r^2p^2 - \phi^2 + i\hbar\,\phi\right) - 2\frac{\mu\kappa}{r}\left(r^2p^2 - \phi^2 + i\hbar\,\phi\right) + \hbar^2p^2 - 2\hbar^2\frac{\mu\kappa}{r} \\
&= (\mu\kappa)^2 + p^2L^2 - 2\frac{\mu\kappa}{r}L^2 + \hbar^2p^2 - 2\hbar^2\frac{\mu\kappa}{r} \\
&= (\mu\kappa)^2 + 2\mu\left(\frac{p^2}{2\mu} - \frac{\kappa}{r}\right)L^2 + 2\mu\hbar^2\left(\frac{p^2}{2\mu} - \frac{\kappa}{r}\right) \\
&= (\mu\kappa)^2 + 2\mu H(L^2 + \hbar^2),
\end{aligned} \tag{6.22}$$

omitting factors of the identity operator I.

6.2.3 Hamiltonian

From the eccentricity, the Hamiltonian

$$H = \frac{p^2}{2\mu} - \frac{\kappa}{r} = -\mu\kappa^2\frac{1-e^2}{2(L^2+\hbar^2)} = H^\dagger. \tag{6.23}$$

The Hamiltonian commutes with the eccentricity and the angular momentum squared

$$[H, e_a] = 0, \tag{6.24a}$$

$$[H, L^2] = 0, \tag{6.24b}$$

as in Problem 3, and the three vector operates obey the commutation relations

$$[L_a, L_b] = i\hbar\,\epsilon_{abc}L_c, \tag{6.25a}$$

$$[L_a, e_b] = i\hbar\,\epsilon_{abc}\,e_c, \tag{6.25b}$$

$$[e_a, e_b] = i\,\epsilon_{abc}\,L_c\left(-2H\hbar^2/\mu\kappa^2\right), \tag{6.25c}$$

as in Problem 4. Restrict the operators to act only on those vectors in the Hilbert space that are eigenstates of the Hamiltonian H, an eigensubspace in which Hamiltonian acts like a number $H = EI$, with $E < 0$, and introduce the scaled eccentricity

$$\vec{\epsilon} = \sqrt{\frac{\mu\kappa^2}{-2E\hbar^2}}\,\vec{e} \tag{6.26}$$

to simplify the Eq. 6.25 commutation relations

$$[L_a, L_b] = i\hbar\,\epsilon_{abc}L_c, \tag{6.27a}$$
$$[L_a, \hbar\epsilon_b] = i\hbar\,\epsilon_{abc}\epsilon_c, \tag{6.27b}$$
$$[\hbar\epsilon_a, \hbar\epsilon_b] = i\hbar\,\epsilon_{abc}L_c, \tag{6.27c}$$

which define a Lie algebra with structure constants $\hbar\epsilon_{abc}$.

Different combinations of basis vectors $\vec{\epsilon}$ and $\vec{L}$ imply different structure constants. "Uncouple" $\vec{\epsilon}$ and $\vec{L}$ by the "rotation"

$$\vec{J}^{\pm} = \frac{\vec{L} \pm \hbar\vec{\epsilon}}{2} \tag{6.28}$$

to further simplify the commutation relations

$$[J_a^+, J_b^-] = 0, \tag{6.29a}$$
$$[J_a^+, J_b^+] = i\hbar\,\epsilon_{abc}J_c^+, \tag{6.29b}$$
$$[J_a^-, J_b^-] = i\hbar\,\epsilon_{abc}J_c^-, \tag{6.29c}$$

and the Hamiltonian

$$H = -\mu\kappa^2\frac{1}{2(4J^2+\hbar^2)}, \tag{6.30}$$

where $J^2 = J^+J^+ = J^-J^-$.

6.2.4 Eigenvalues

Since J obey the angular momentum commutation relations, there exist states states $|j\rangle$ such that

$$J^2|j\rangle = j(j+1)\hbar^2|j\rangle, \tag{6.31}$$

for $j = 0, 1/2, 1, 3/2, 2, \ldots$. Since $[H, J^2] = 0$, there exist states $|E, j\rangle$ such that

$$H|E,j\rangle = E|E,j\rangle, \tag{6.32a}$$
$$J^2|E,j\rangle = j(j+1)\hbar^2|E,j\rangle, \tag{6.32b}$$

If the state $|\psi\rangle$ is in the space spanned by these states, then

$$H|\psi\rangle = -\mu\kappa^2\frac{1}{2(4J^2+\hbar^2)}|\psi\rangle \tag{6.33}$$

and

$$E|\psi\rangle = -\mu\kappa^2\frac{1}{2(4j(j+1)\hbar^2+\hbar^2)}|\psi\rangle. \tag{6.34}$$

Since this is true for all such states,

$$E = -\frac{\mu\kappa^2}{2(2j+1)^2\hbar^2} < 0 \tag{6.35}$$

or

$$E_n = \frac{E_1}{n^2} < 0, \tag{6.36}$$

where the ground state

$$E_1 = -\frac{\mu\kappa^2}{2\hbar^2} = -\frac{1}{2}m_e c^2\left(k\frac{q_e^2}{\hbar c}\right)^2 \approx -\frac{1}{2}\,511\text{ keV}\left(\frac{1}{137}\right)^2 = -13.6\text{ eV}, \tag{6.37}$$

for $n = 2j+1 = 1, 2, 3, \ldots$.

Problems

1. Let Q and P be position and momentum operators satisfying $[Q, P] = i\hbar I = i\hbar$. Derive the following commutators.
   (a) $[Q, P^2] = 2i\hbar P$.
   (b) $[Q, P^n] = ni\hbar P^{n-1}$.
   (c) $[Q, f[P]] = i\hbar f'[P] = i\hbar\, df/dP$.
   (d) $[P, f[Q]] = -i\hbar f'[Q] = -i\hbar\, df/dQ$.
2. Derive the Table 6.1 commutators.
3. Verify the Eq. 6.24 commutators.
4. Verify the Eq. 6.25 commutators.

Appendix A

Notation

Table A.1 summarizes the symbols of this text. Some symbols are more universal than others.

Table A.1: Symbols used in this text.

Quantity	Symbol	Alternates
state	$\|\psi\rangle, \|\psi_t\rangle$	Ψ
unitary operator	U	
hermitian operator	H	
time translation	T, T'	S_t
space translation	S_a, S'_a	S_a
space rotation	R_a, R'_a	$R_{\vec{\theta}}$
boost	B_a, B'_a	G_a
coordinates	x_a, x, y, z, t	
small change	ϵ, δ	
position operator	Q_a	X_a, r_a
momentum operator	P_a	p_a
velocity operator	V_a	v_a
angular momentum operator	$J_a, J_a, \mathscr{S}_a$	
Hamiltonian energy operator	H	

Standard mathematics notation suffers from a serious ambiguity involving parentheses. In particular, parentheses can be used to denote multiplication, as in $a(b+c) = ab + ac$ and $f(g) = fg$, or they can be used to denote functions evaluated at arguments, as in $f(t)$ and $g(b+c)$. It can be a struggle to determine the intended meaning from context.

To avoid ambiguity, this text always uses round parentheses $(\bullet)$ to group for multiplication and square brackets $[\bullet]$ to list function arguments. Thus, $a(b) = ab$ denotes the product of two factors a and b, while $f[x]$ denotes a function f evaluated at an argument x. *Mathematica* [13] employs the same convention.

Appendix B

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