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QUANTUM TECHNOLOGIES

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DIGITALLY ENHANCED QUANTUM TECHNOLOGY MASTER

QUANTUM TECHNOLOGIES

The principles of quantum mechanics, which govern physics, chemistry, material science and computing at the nanoscale are leading a wave of new technologies which have the potential to revolutionize how we communicate, process information and learn about our world. This course aims to give you the tools to understand, develop and apply quantum technologies, enabling you to be part of the second quantum revolution.

While primarily targeting physics students, the course is also designed to be accessible to engineering, mathematics or computer science students seeking a deeper understanding of underlying principles.

Part A: Concepts and Foundations

- Learn the historical context leading to the first and second quantum revolutions.
- Review the core concepts and foundations of quantum mechanics.
- Explore how to manipulate quantum systems using light.

Part B: Physical Platforms

- Dive into the design and operation of superconducting qubits.
- Learn how to prepare and control atomic quantum systems.
- Understand how photons can be used to encode, transmit and process quantum information.

Part C: Applications (under construction)

- Get to know quantum computing and its capabilities.
- Explore applications in quantum sensing, communication, and simulation.
- Discover multidisciplinary applications of quantum technologies.

Contents

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QUANTUM: THE SECOND REVOLUTION

Concepts and Foundations

This chapter provides a historical overview of the evolution of quantum mechanics, from the first quantum revolution, which introduced transformative technologies like transistors and lasers that underpin the modern information age, to the second quantum revolution, which aims to harness quantum effects such as entanglement for future technologies. It summarizes key quantum principles, including quantization, superposition, and entanglement, which form the foundation for quantum technologies. The chapter concludes with the DiVincenzo criteria, a framework for evaluating various technological platforms, setting the stage for a comparative analysis of quantum technologies in the subsequent chapters.

Key points:

- Historical evolution of quantum theory
- Quantum principles
- First and second quantum revolution
- Divincenzo criteria

Good resources for this chapter include:

- History of Quantum Theory (August 10, 2024). In Wikipedia. https://en.wikipedia.org/w/index.php?title=History_of_quantum_mechanics&oldid=1239610407
- Quantum Technology, the Second Quantum Revolution by Dowling and Milburn, Phil. Trans. R. Soc. A.3611655–1674 (2003).

Timeline: Major Milestones in Quantum Science and Technology

- 1865: Maxwell unifies electricity, magnetism, and light
- 1900: Planck proposes quantization of energy
- 1905: Einstein explains the photoelectric effect using light quanta (photons)
- 1913: Bohr's quantized model of the atom
- 1922: Stern–Gerlach demonstrates quantized spin
- 1924: de Broglie introduces matter waves
- 1925–26: Heisenberg, Schrödinger, and Dirac formalize quantum mechanics
- 1927: Davisson–Germer experimentally confirm electron waves; Fifth Solvay Conference debates foundations
- 1935: Einstein–Podolsky–Rosen (EPR) paradox and Schrödinger's cat highlight entanglement
- 1947: Invention of the transistor
- 1954/1960: Maser and then laser invented
- 1982: Aspect et al. experimentally confirm quantum nonlocality
- 1994: Shor's quantum factoring algorithm
- 2019: Google Sycamore evidence for a quantum computational advantage

1.1 Origin story: The Birth of Quantum Mechanics

In the late 19th century, classical physics had achieved substantial successes in describing natural phenomena, leading many to believe that the fundamental principles governing nature were nearly complete. However, a series of puzzling experimental results at the

turn of the 20th century challenged this view, revealing fundamental limitations of classical theory and highlighting the need for a new scientific worldview. These discoveries laid the groundwork for quantum mechanics and marked the onset of what is now called the first quantum revolution, a scientific transformation which underpins many of the transformative technologies of the twentieth century.

Maxwell's electromagnetism

In 1865, James Clerk Maxwell formulated the classical theory of electromagnetic radiation, describing how electric and magnetic fields interact and propagate as waves. Maxwell's theory unified electricity, magnetism, and light, and its wave-based formalism set the stage for a new understanding of nature. Whereas classical waves represent physical oscillations of fields, quantum wavefunctions describe probability amplitudes for measurement outcomes and do not correspond to directly observable physical quantities.

Maxwell's equations were so successful that by the late 19th century, many physicists believed that classical physics had nearly reached its limits. This optimism is often encapsulated in a statement, commonly misattributed to Lord Kelvin but more likely representative of the prevailing view among physicists before the quantum era:

> "There is nothing new to be discovered in physics now, only more precise measurements."

However, this belief was soon to be challenged by experimental evidence that classical theories could not explain.

Planck's quantum hypothesis

At the turn of the 20th century, Max Planck made a groundbreaking discovery while attempting to explain the energy spectrum of black-body radiation and the so-called "ultraviolet catastrophe" predicted by the Rayleigh–Jeans law, but contradicted by experiments. In 1900, he proposed that electromagnetic energy is emitted in discrete units, or "quanta," leading to the famous relationship

$$E = h\nu,$$

where E is the quantum of energy, ν is the frequency, and h is Planck's constant. Planck's hypothesis was initially a pragmatic attempt to fit experimental data, and was only later recognized as a radical departure from classical physics.

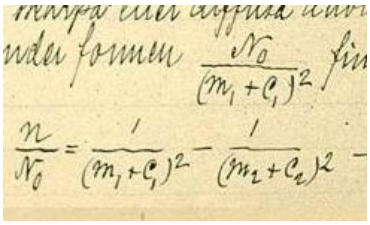

Figure 1.1: The original Rydberg formula expresses the wavenumber n of spectral lines. In this formula, N_0 is a constant, while m_1 and m_2 are two integers. The values c_1 and c_2 are numbers that depend on the atomic species and the specific spectral series. Today, we recognize N_0 as the Rydberg constant, m_1 and m_2 as principal quantum numbers, and c_1 and c_2 as quantum defects.

Planck's constant was later defined as an exact number

$$h = 6.62607015 \times 10^{-34}\,\text{Js}$$

with the redefinition of the International System of Units (SI) in 2019, which also led to the redefinition of other units, such as the kilogram, in terms of fundamental constants.

Bohr model of the atom

Not long after, in 1913, Niels Bohr developed his quantum model of the atom to explain the empirical Rydberg formula for hydrogen's spectral lines, observed both in laboratory discharge tube spectra and in the astronomical spectra of stars. Bohr proposed that electrons move in quantized orbits around the nucleus and emit or absorb light only when jumping between these orbits. Although later superseded, the Bohr model was a landmark, as it explained atomic stability and spectra using quantization principles unaccounted for by classical models.

The dawn of quantum theory

By the 1920s, quantum theory was advancing rapidly. In 1924, Louis de Broglie proposed that matter, like light, exhibits both wave and particle characteristics, introducing the concept of "matter waves" and the de Broglie wavelength. This insight laid the groundwork for Schrödinger's wave mechanics and further cemented the principle of wave-particle duality. The subsequent formulation of matrix mechanics by Heisenberg, wave mechanics by Schrödinger, and their probabilistic interpretation by Born culminated in the modern framework of quantum mechanics. In 1927, the Fifth Solvay Conference brought together

Einstein, Bohr, Heisenberg, Schrödinger, de Broglie, and others for far-reaching debates on the interpretation of quantum phenomena and wave-particle duality. Key experiments such as Stern–Gerlach (1922, spin quantization) and Davisson–Germer (1927, electron diffraction) gave direct confirmation to the quantum theory. The Copenhagen interpretation, which posits that quantum systems exist in a superposition of states until measured, became dominant. Nevertheless, philosophical debates about completeness (the EPR paradox), measurement, and reality persist to this day.

1.2 Quantum Principles

Quantum technologies aim to deliver useful devices and processes based on quantum principles, which include:

Quantization of energy

In quantum mechanics, the allowed energies of a confined system are restricted to discrete sets. For example, for an electron in a hydrogen atom:

$$E_n = -\frac{13.6\,\text{eV}}{n^2},$$

where n is a principal quantum number, and 13.6 eV is the ionization energy for hydrogen.

Superposition principle

The superposition principle states that a quantum system can exist in multiple states simultaneously until a measurement is made. For example a general state $|\psi\rangle$ can be written:

$$|\psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle$$

with $|c_0|^2 + |c_1|^2 = 1$. Unlike classical probabilities, which reflect incomplete knowledge of an underlying state, quantum measurement outcomes are intrinsically probabilistic. The superposition principle is famously illustrated by Schrödinger's cat, which is described as both alive and dead until observed.

Wavefunction collapse and measurement

The wavefunction describes the quantum state of a system; measurement causes the wavefunction to "collapse" to a single outcome, discarding all other possibilities.

Heisenberg's Uncertainty Principle

Heisenberg's uncertainty principle asserts that certain pairs of observables cannot both be known with arbitrary precision:

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

where Δx and Δp are, respectively, the uncertainties in position and momentum.

Wave-particle duality

Wave-particle duality describes how light and matter both display wave and particle properties. Young's double-slit experiment demonstrated light's wave nature, while the photoelectric effect revealed its quantum, particle-like aspect. Louis de Broglie extended this idea to matter, proposing:

$$\lambda = \frac{h}{mv},$$

a relation directly validated in the Davisson–Germer experiment in 1927, which confirmed that electrons exhibit wave behavior with a wavelength given by the de Broglie relation, a principle routinely exploited today in electron microscopes, atom interferometers, and studies of ultracold matter (e.g., Bose–Einstein condensates).

Quantum entanglement and nonlocality

Quantum entanglement extends the superposition principle to composite systems, creating correlations that persist regardless of spatial separation. The EPR paradox (1935) famously questioned quantum completeness and locality, leading to foundational advances. Alain Aspect's experiments (1982), using entangled photons, confirmed violations of Bell inequalities, cementing nonlocal correlations at the heart of quantum theory and enabling applications in quantum communication and computation.

1.3 The first quantum revolution

The first quantum revolution concerned the development of quantum mechanics as a scientific theory, fundamentally transforming the understanding of nature at microscopic scales and spawning technologies that anchor the contemporary information society.

- *Development of Transistors:* The transistor, invented in 1947 by John Bardeen, Walter Brattain, and William Shockley, is the basic building block of modern electronics. Transistors harness quantum principles such as energy quantization and band structure to control electronic signals.
- *Atomic Clocks and GPS:* Atomic clocks, developed in the 1950s, use quantum transitions of atoms for ultra-precise timekeeping, a prerequisite for satellite navigation and global positioning.
- *Nuclear Magnetic Resonance (NMR):* NMR, discovered in the 1940s, utilizes quantum spin resonance for detailed molecular analysis and forms the basis for MRI.
- *The laser:* The laser, invented in 1960, exploits stimulated emission for generating coherent light. Once termed "a solution in search of a problem," lasers now pervade telecommunications, medicine, and quantum optics. The maser (microwave amplification by stimulated emission of radiation, 1954) is the precursor to the laser and similarly exploits quantum effects.

1.4 Entering a New Quantum Age

The first quantum revolution provided new theoretical tools and foundational technologies. The second quantum revolution, ongoing today, is defined by the engineered exploitation of quantum phenomena such as superposition and entanglement, enabling new technological applications.

Quantum simulation

Originally envisioned by Richard Feynman in 1982, in his seminal paper "Simulating Physics with Computers," quantum simulators are physical systems engineered to mimic other quantum systems or classes of models by reproducing their Hamiltonians as closely as possible. Feynman argued that certain quantum systems cannot be efficiently simulated by classical computers, and that controllable quantum devices built from atoms, ions,

photons, or other quantum platforms, could naturally model the complex dynamics of interacting particles. Quantum simulators are typically used to study phenomena such as electron behavior in solids, magnetism, quantum phase transitions, high-temperature superconductivity, and even aspects of quantum chemistry and lattice gauge theories.

Quantum Computing

Quantum computers encode information using quantum bits (qubits) and process it by applying quantum gates—unitary operations acting on single or multiple qubits that form the building blocks of quantum circuits. This framework enables fundamentally new algorithms, such as Shor's algorithm for efficient integer factorization, which is believed to be intractable on conventional computers. Recent experiments, including Google's Sycamore processor in 2019, have demonstrated quantum computational advantage for certain benchmark tasks, though some results remain debated in light of advances in classical simulation methods. Nevertheless, rapid progress in hardware strongly suggests that quantum advantage for specific classes of problems may soon be practically realized.

Quantum Sensing and Metrology

Quantum sensors harness phenomena such as superposition, entanglement, and squeezing to measure physical quantities with precision beyond classical limits. Applications include atomic clocks for ultra-precise timekeeping, magnetometers for sensitive detection of magnetic fields, quantum-enhanced interferometers for gravitational wave detection, and a new generation of devices for inertial navigation and imaging.

Quantum Communication

Quantum communication leverages principles like entanglement and the no-cloning theorem to enable provably secure information transfer. Protocols such as quantum key distribution (QKD) can detect eavesdropping and guarantee the security of cryptographic keys. Ongoing developments include satellite-based quantum links and quantum repeater technologies, forming the building blocks for robust quantum networks and the envisioned quantum internet.

1.5 The Divincenzo Criteria

As theoretical ideas transition into practical technologies, robust criteria for evaluating physical implementations are essential. Although originally articulated for quantum computing, the DiVincenzo criteria offer a valuable framework for comparing platforms across quantum technology. In the following chapters, we use these criteria as a foundation for comparative analysis.

1. *Quantum system:* Scalable physical system with well-defined qubits
2. *Initialization:* Ability to initialize the state of the qubits to a simple fiducial state
3. *Coherence:* Long relevant decoherence times
4. *Interactions:* A "Universal" set of quantum gates
5. *Measurement:* Qubit specific measurement capabilities

Two additional criteria relate specifically to quantum communication:

1. *Interconversion:* The ability to interconvert stationary and flying qubits
2. *Transmission:* The ability to faithfully transmit flying qubits between specified locations

Through these criteria, we can effectively compare different technologies and identify the essential capabilities required for the coming era of quantum engineering.

Exercises

Exercise 1.1

Using the Heisenberg uncertainty principle, estimate the characteristic length scale where quantum effects become important for:

1. *An electron at room temperature*
2. *A potassium atom cooled to a temperature of 1 millionth of a degree above absolute zero*

Exercise 1.2

- *Describe a scenario, ideally including a physical setup, in which quantum measurements could be used to generate random numbers. Identify various applications where this could be useful.*

The Shannon entropy quantifies the amount of information or uncertainty in a random variable. For a discrete random variable X with possible outcomes x_i and corresponding probabilities $p(x_i)$, the Shannon entropy is:

$$H(X) = -\sum_i p(x_i) \log_2(p(x_i))$$

- *For an ideal implementation of your QRNG design, calculate the theoretical maximum Shannon entropy per measurement.*
- *What effects might diminish the entropy of your quantum random number generator?*

Exercise 1.3

Niels Bohr proposed a theoretical model for the atom that provided a physical basis for Rydberg's formula. Bohr hypothesised that an atom consists of a small, positively charged nucleus surrounded by electrons which travel in elliptical orbits with quantized angular momentum:

$$r \times m_e v = n\hbar, \tag{1.1}$$

where m_e is the electron mass and v is the electron velocity and n is a positive integer. Discrete spectral lines then correspond to jumps of the electron between orbits with different n.

- *Write expressions for the centripetal force acting on the electron and the Coulomb force between the electron and the nucleus.*
- *Equate these forces and solve for the electron's orbital radius r as a function of n.*
- *Identify the scaling relationship between r and n?*
- *Check the units of your expression for r. What is the prefactor?*

2

QUANTUM CONCEPTS

Concepts and Foundations

Quantum information theory is a framework that helps us grasp how quantum systems can process and transmit information in ways that classical systems simply cannot. In this lecture, we will introduce the necessary notation and review the key concepts and mathematical tools that form the foundation for quantum technologies.

Key points:

- Quantum mechanics of discrete systems
- Quantum states and operators
- Pure and mixed states
- Time evolution
- Approximation methods

A good resource for this chapter is:

- Nielsen and Chuang, *Quantum Computation and Quantum Information*, in particular Sections 2.1 and 2.2.

2.1 The State Vector

Quantum mechanics provides a comprehensive framework for understanding the behavior of physical systems at the smallest scales. The theory is built upon several key postulates that define how quantum systems are described, how measurements are made, and how systems evolve over time.

States

A quantum system is specified by a state vector in a Hilbert space, a complex vector space with an inner product. The state vector, often denoted as $|\psi\rangle$, contains all the information about the system. In Dirac notation, state vectors are represented by ket's (and bra's, the vector dual of a ket).

$$|\psi\rangle = \text{“ket”}$$
$$\langle\psi| = \text{“bra”}$$

The **norm-square** of a state vector is given by the inner product with itself.

$$\|\psi\|^2 = \langle\psi|\psi\rangle$$

The *normalization* condition is $\|\psi\|^2 = 1$ which ensures that the total probability of all possible measurement outcomes is 1.

In general

$$\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^* \in \mathbb{C}$$

Hilbert Space

Quantum states are elements of a linear vector space called the Hilbert space. Linear combinations of state vectors are also elements of the same Hilbert space.

$$|\psi_1\rangle + |\psi_2\rangle \in \mathcal{H}, \quad a|\psi\rangle \in \mathcal{H}, \quad a \in \mathbb{C}$$

Complete Orthonormal Basis

A set of vectors $\{|1\rangle, |2\rangle, \ldots, |d\rangle\}$ that are mutually orthogonal and normalized, i.e.:

$$\langle i|j\rangle = \delta_{ij},$$

constitutes an orthonormal basis.

A set of orthonormal vectors forms a **complete orthonormal basis** if any vector in the Hilbert space can be expressed as a linear combination of these vectors.

$$\forall|\phi\rangle \in \mathcal{H}, \quad |\phi\rangle = \sum_j c_j|j\rangle$$

The *completeness relation* expresses that a complete orthonormal basis spans the entire Hilbert space

$$\sum_j |j\rangle\langle j| = \mathbb{1}$$

Qubit Example: Two-State System

A qubit is the simplest quantum system, analogous to a classical bit but with the possibility to occupy a superposition of two states.

$$\text{Basis: } \{|0\rangle, |1\rangle\} \to |\psi\rangle = c_0|0\rangle + c_1|1\rangle, \quad |c_0|^2 + |c_1|^2 = 1.$$

Alternatively, in the $\{|+\rangle, |-\rangle\}$ basis, with $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$,

$$|\psi\rangle = d_+|+\rangle + d_-|-\rangle,$$

where $d_+ = (c_0 + c_1)/\sqrt{2}$, $d_- = (c_0 - c_1)/\sqrt{2}$.

2.2 Operators

Linear Operators

Operators act on state vectors to produce new state vectors.

$$|\psi\rangle \mapsto |\psi'\rangle = \hat{A}|\psi\rangle$$

Operators are linear and distributive.

$$\hat{A}(a|\psi\rangle + b|\phi\rangle) = a\hat{A}|\psi\rangle + b\hat{A}|\phi\rangle$$

The matrix elements of an operator can be expressed as:

$$A_{mn} = \langle m|\hat{A}|n\rangle$$

An operator can be expressed in braket form using the completeness relation

$$\hat{A} = \sum_{m,n} A_{mn} |m\rangle \langle n|$$

Hermitian and Unitary Operators

$$\begin{aligned} &\text{Unitary:} \quad \hat{U}^\dagger = \hat{U}^{-1}, \quad \hat{U}^\dagger\hat{U} = 1 \\ &\text{Hermitian:} \quad \hat{A} = \hat{A}^\dagger, \quad A_{mn} = A^*_{nm} \end{aligned}$$

Time-evolution of closed quantum systems are described by unitary operators (norm preserving and reversible). Observables are described by hermitian operators. Hermitian operators have real eigenvalues corresponding to possible measurement outcomes.

Spectral Decomposition

Any Hermitian operator can be expressed in terms of its eigenvalues and eigenvectors.

$$\hat{A} = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$$

$\{|\phi_i\rangle\}$ is an orthonormal basis (ONB).

Qubit Example: Pauli Operators

Pauli operators are fundamental in describing qubit operations:

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

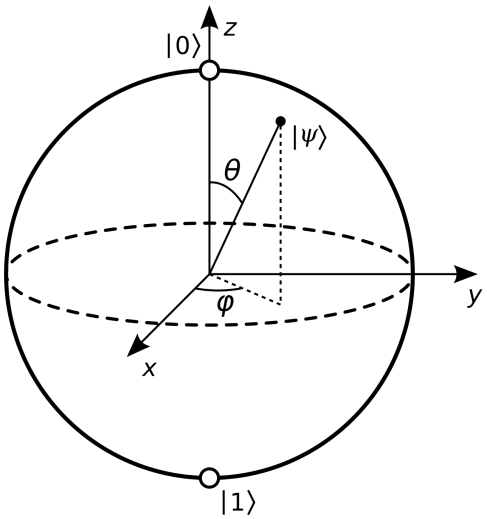

Figure 2.1: Bloch sphere.

Bloch sphere representation

The Bloch sphere representation is a powerful geometric visualization of a two-level system in quantum mechanics.

A general qubit state can be expressed as:

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

where θ and ϕ are spherical coordinates. The Bloch sphere is a unit sphere where the state of a qubit can be described by a vector $\vec{r} = (x, y, z)$, where:

$$x = \langle\psi|\hat{\sigma}_x|\psi\rangle = \langle\hat{\sigma}_x\rangle, \quad y = \langle\hat{\sigma}_y\rangle, \quad z = \langle\hat{\sigma}_z\rangle$$

- The north pole represents the state $|0\rangle$, since $\langle 0|\hat{\sigma}_z|0\rangle = +1$.
- The south pole represents the state $|1\rangle$, since $\langle 1|\hat{\sigma}_z|1\rangle = -1$.
- Any other point on the sphere represents a superposition of $|0\rangle$ and $|1\rangle$.

The length of the vector $\vec{r}$ is always 1 for pure states due to normalization (the Bloch vector lives on the surface of the Bloch sphere). For mixed states, the Bloch vector may be thought of as living inside the sphere (i.e., its length is less than 1).

Single qubit manipulations are described by unitary operators, e.g.,

$$\hat{U} = e^{i\Theta\hat{\sigma}_j},$$

corresponds to a rotation on the Bloch sphere by an angle Θ around the rotation axis j.

2.3 Measurements

In quantum mechanics, physical observables are represented by Hermitian operators.

- The possible outcomes of a measurement correspond to the eigenvalues of these operators
- The state of the system collapses to the corresponding eigenstate upon measurement.
- The probability of obtaining a particular measurement outcome is determined by the projection of the state vector onto the eigenstate, i.e. $P_\alpha = |\langle\alpha|\psi\rangle|^2$

Expectation Values

The expectation value of an observable $\hat{A}$ in a state $|\psi\rangle$ is given by the eigenvalues a of $\hat{A}$ weighted by the probability of obtaining outcome a:

$$\langle\hat{A}\rangle = \sum_a aP(a) = \langle\psi|\hat{A}|\psi\rangle$$

$$\hat{A}|\psi_a\rangle = a|\psi_a\rangle$$
$$P(a) = |\langle\psi_a|\psi\rangle|^2$$

2.4 Dynamics

The time evolution of a quantum system is governed by Schrödinger's equation. The Hamiltonian operator $\hat{H}$ represents the total energy of the system and dictates how the state vector changes over time.

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle$$

Note: For a time-independent Hamiltonian, the solution to Schrödinger's equation can be expressed as:

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t}|\psi_0\rangle, \quad |\psi(0)\rangle = |\psi_0\rangle$$

Basis Set Expansion

Expressing the state vector in terms of a basis set simplifies the analysis of time evolution.

$$|\psi(t)\rangle = \sum_j c_j(t)|j\rangle \rightarrow i\hbar\dot{c}_j(t) = \sum_i H_{ji}c_i(t)$$

Functions of Operators

Functions of operators can be expanded similarly to scalar functions.

$$f(\hat{H}) = \sum_n \alpha_n \hat{H}^n$$

A common example is the exponential of an operator, which can be expressed as a Taylor series:

$$e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{1}{n!}\hat{A}^n = 1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \frac{1}{3!}\hat{A}^3 + \cdots$$

For example,

$$\begin{aligned} |\psi(t)\rangle &= e^{-\frac{i}{\hbar}\hat{H}t}\,|\psi_0\rangle \\ &= e^{-\frac{i}{\hbar}\hat{H}t}\sum_j |\phi_j\rangle\langle\phi_j|\psi_0\rangle \end{aligned}$$

Here, we can expand the exponential operator using its Taylor series:

$$\begin{aligned} e^{-\frac{i}{\hbar}\hat{H}t} &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\hat{H}t\right)^n \\ &= 1 - \frac{i}{\hbar}\hat{H}t + \frac{1}{2!}\left(-\frac{i}{\hbar}\hat{H}t\right)^2 + \frac{1}{3!}\left(-\frac{i}{\hbar}\hat{H}t\right)^3 + \cdots \end{aligned}$$

When this operator acts on an energy eigenstate $|\phi_j\rangle$, we get:

$$\begin{aligned} e^{-\frac{i}{\hbar}\hat{H}t}|\phi_j\rangle &= \left[1 - \frac{i}{\hbar}E_j t + \frac{1}{2!}\left(-\frac{i}{\hbar}E_j t\right)^2 + \cdots\right]|\phi_j\rangle \\ &= e^{-iE_j t/\hbar}|\phi_j\rangle \end{aligned}$$

Combining this we obtain:

$$|\psi(t)\rangle = \sum_j e^{-iE_j t/\hbar}\langle\phi_j|\psi_0\rangle|\phi_j\rangle$$

Qubit Example: Free Evolution

Consider a qubit with a Hamiltonian $\hat{H} = \hbar\omega\hat{\sigma}_z$, where ω is a frequency parameter. The eigenstates of σ_z are $|0\rangle$ and $|1\rangle$. Suppose the qubit starts in the state $|\psi_0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$. Then the solution is:

$$e^{-\frac{i}{\hbar}\hat{H}t}|\psi_0\rangle = \frac{1}{\sqrt{2}}(e^{-i\omega t}|0\rangle + e^{i\omega t}|1\rangle)$$

This represents a rotation of the qubit's state about the z-axis of the Bloch sphere.

2.5 Uncertainty

In classical physics, properties of objects are assumed to have definite values independent of observation. However, quantum mechanics challenges this intuition by asserting that certain properties cannot simultaneously take definite values. Measurements generally alter the state of the system.

For example, consider measuring the $\hat{\sigma}_x$ operator on a quantum state initially prepared in the eigenstate $|0\rangle$ of the σ_z operator. The measurement outcomes are random, with probabilities determined by the overlap of $|0\rangle$ with the eigenstates of σ_x. Each outcome (corresponding to the eigenstates of σ_x $\frac{|0\rangle \pm |1\rangle}{\sqrt{2}}$) occurs with probability 50%.

Mathematically, this is expressed by the non-commutativity of operators. Two operators are not simultaneously diagonalizable if they do not commute, as shown by:

$$[\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y$$

2.6 Entanglement

Entanglement is a uniquely quantum mechanical phenomenon where the states of two or more quantum objects or subsystems become interconnected. This is represented using tensor products. Consider two qubits with basis states $|00\rangle, |01\rangle, |10\rangle, |11\rangle$.

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B \quad \mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$$

For example, in coefficient notation:

$$|\psi\rangle_A = a_0|0\rangle + a_1|1\rangle$$
$$|\psi\rangle_B = b_0|0\rangle + b_1|1\rangle$$
$$|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B \equiv |\psi_A\psi_B\rangle$$
$$\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \otimes \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} a_0 b_0 \\ a_0 b_1 \\ a_1 b_0 \\ a_1 b_1 \end{pmatrix}$$

Separable states are of the form $|\psi\rangle_{AB} = |\psi\rangle_A \otimes |\psi\rangle_B$. All other states are entangled.

Example: The singlet state

$$|\psi_{AB}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

2.7 The Density Operator

So far we have considered pure quantum states represented by a statevector $|\psi\rangle$. However in real world situations interactions with the environment or incomplete information about the system leads to mixed states.

A mixed state can be thought of as a statistical mixture of pure states with classical probabilities p_i. It is described by the **density operator** or **density matrix**

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

A pure state can also be represented as a density operator $\hat{\rho}_{\text{pure}} = |\psi\rangle\langle\psi|$.

The purity of a quantum state is defined by the trace $\text{Tr}(\hat{\rho}^2) \leq 1$. (For a pure state, $\text{Tr}(\hat{\rho}^2) = 1$)

The density operator has the following properties:

1. Hermiticity $\hat{\rho} = \hat{\rho}^\dagger$
2. Trace one $\text{Tr}(\hat{\rho}) = 1$ (normalization condition)
3. Positivity $\langle\phi|\hat{\rho}|\phi\rangle \geq 0$ (for any state $|\phi\rangle$)

The density operator can be expressed as a matrix where the elements are:

$$\rho_{\alpha\beta} = \langle\alpha|\hat{\rho}|\beta\rangle$$

The diagonal elements of the density matrix ρ_{ii} are called **probabilities**: the probabilities of finding the system in the state $|\psi_i\rangle$. The off diagonal elements of the density matrix are called **coherences**.

Partial trace

The partial trace is an operation used to extract the state of a subsystem from a larger composite system. Consider the bipartite system described by a Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The partial trace over system B gives the reduced density operator for system A

$$\hat{\rho}_A = \mathrm{Tr}_B(\hat{\rho}_{AB}) = \sum_i \langle b_i|\hat{\rho}_{AB}|b_i\rangle$$

Here, $\hat{\rho}_{AB}$ denotes the density operator of the full system, and $\{|b_i\rangle\}$ is an orthonormal basis of subsystem B.

The partial trace can be interpreted as an averaging over all possible states for subsystem B.

Qubit example: Entanglement leads to mixed states

The loss of purity of a quantum state can be understood as a consequence of information loss, or entanglement of the system with environmental degrees of freedom.

To illustrate, consider two qubits in a pure entangled state

$$\hat{\rho} = |\psi\rangle\langle\psi|, \quad \text{where } |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_1|1\rangle_2 - |1\rangle_1|0\rangle_2\right)$$

where we use the subscript indices to explicitly keep track of the two subsystems.

The reduced density matrix for the first qubit $\hat{\rho}_1$ is

$$\hat{\rho}_1 = \sum_{j=\{0,1\}} \langle j|\hat{\rho}|j\rangle_2$$

$$\begin{aligned}\hat{\rho}_1 &= \langle 0|\hat{\rho}|0\rangle_2 + \langle 1|\hat{\rho}|1\rangle_2 \\ &= \frac{1}{2}|0\rangle_1\langle 0| + \frac{1}{2}|1\rangle_1\langle 1|\end{aligned}$$

This describes a fully mixed state with $\mathrm{Tr}(\hat{\rho}_1^2) = \frac{1}{2}$. Measurements on the first qubit would yield random outcomes consistent with a statistical mixture (no coherences).

Dynamics of the density operator

The time-evolution of the density operator follows from the Schrödinger equation applied to each state comprising the statistical mixture. The resulting equation of motion is called the **Liouville-von Neumann equation**

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[H, \hat{\rho}]$$

In general however, the time-evolution of the density operator can also be influenced by environmental degrees of freedom. Often assumptions are made about the environment, e.g., that fluctuations of the environment are Markovian (memoryless) and that the system-bath coupling is weak. Tracing out these degrees of freedom leads to a general form for the quantum master equation called the **Lindblad Master equation**:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[H, \hat{\rho}] + \sum_j \hat{L}_j\hat{\rho}\hat{L}_j^\dagger - (\hat{L}_j^\dagger\hat{L}_j\hat{\rho} + \hat{\rho}\hat{L}_j^\dagger\hat{L}_j)/2$$

where $\hat{L}_j$ is a set of jump operators describing the dissipative processes. $\hat{L}_j$ do not need to be unitary operators. For example the jump operator $\hat{L} = \sqrt{\Gamma}\hat{\sigma}^-$ describes a process with a rate Γ which involves a transition from a higher energy state to a lower energy state, such as spontaneous emission in a two-level atom.

2.8 Approximation methods in quantum mechanics

Approximation methods are essential tools in quantum mechanics for solving complex problems that lack exact analytical solutions. These methods often involve perturbative approaches, where a system is divided into solvable or known parts and and small perturbative parts.

2.8.1 Time-Independent Perturbation Theory

In perturbation theory, we separate the Hamiltonian into an unperturbed part $\hat{H}_0$ and a perturbation $\lambda\hat{V}$:

$$\hat{H} = \hat{H}_0 + \lambda\hat{V} \tag{2.1}$$

where λ is a small parameter. The energy and eigenvectors are then expanded in powers of λ:

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \tag{2.2}$$

$$|\phi_n\rangle = |\phi_n^{(0)}\rangle + \lambda\,|\phi_n^{(1)}\rangle + \lambda^2\,|\phi_n^{(2)}\rangle + \dots \tag{2.3}$$

Substituting these expansions into the time-independent Schrödinger equation and equating terms of the same order in λ yields:

- Zeroth order: $\hat{H}_0\,|\phi_n^{(0)}\rangle = E_n^{(0)}\,|\phi_n^{(0)}\rangle$
- First order: $\hat{H}_0\,|\phi_n^{(1)}\rangle + \hat{V}\,|\phi_n^{(0)}\rangle = E_n^{(0)}\,|\phi_n^{(1)}\rangle + E_n^{(1)}\,|\phi_n^{(0)}\rangle$
- Second order: $\hat{H}_0\,|\phi_n^{(2)}\rangle + \hat{V}\,|\phi_n^{(1)}\rangle = E_n^{(0)}\,|\phi_n^{(2)}\rangle + E_n^{(1)}\,|\phi_n^{(1)}\rangle + E_n^{(2)}\,|\phi_n^{(0)}\rangle$

For *non-degenerate states*, the first-order energy correction is given by:

$$E_n^{(1)} = \langle\phi_n^{(0)}|\,\hat{V}\,|\phi_n^{(0)}\rangle \tag{2.4}$$

The first-order correction to the eigenstate is:

$$|\phi_n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle\phi_m^{(0)}|\,\hat{V}\,|\phi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}\,|\phi_m^{(0)}\rangle \tag{2.5}$$

The second-order energy correction is:

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\,\langle\phi_m^{(0)}|\,\hat{V}\,|\phi_n^{(0)}\rangle\,|^2}{E_n^{(0)} - E_m^{(0)}} \tag{2.6}$$

For *degenerate states*, the perturbation theory must be adapted by diagonalizing the perturbation within the degenerate subspace.

2.8.2 Adiabatic Elimination

Adiabatic elimination is a technique used to simplify quantum master equations by eliminating fast-evolving degrees of freedom. For example, we can consider a two-level system described by a master equation:

$$\dot{\rho}_{11} = -i\Omega(\rho_{01} - \rho_{01}^*) - \Gamma\rho_{11} \tag{2.7}$$

$$\dot{\rho}_{01} = -i\Omega(\rho_{11} - \rho_{00}) - \frac{\Gamma}{2}\rho_{01} \tag{2.8}$$

$$\tag{2.9}$$

To adiabatically eliminate ρ_{01}, we assume $\dot{\rho}_{01} \approx 0$ (slow evolution compared to other timescales):

$$0 \approx -i\Omega(\rho_{11} - \rho_{00}) - \frac{\Gamma}{2}\rho_{01} \tag{2.10}$$

Solving for ρ_{01}:

$$\rho_{01} \approx \frac{-2\Omega(\rho_{11} - \rho_{00})}{\Gamma} \tag{2.11}$$

This expression can be substituted back into the equations for $\dot{\rho}_{11}$ and $\dot{\rho}_{00}$ to obtain an effective equation for the slow population dynamics.

2.9 Schrieffer-Wolff Transformation

The Schrieffer-Wolff transformation is used to derive effective Hamiltonians for slow degrees of freedom by systematically eliminating high-energy states. We can use subspace projectors P and Q, where P projects onto the low-energy subspace (slow degrees of freedom) and Q = 1 - P projects onto the high-energy subspace (fast degrees of freedom). In general, the equation of motion can be separated into low-energy and high-energy parts:

$$i\dot{\alpha} = P\hat{H}P\alpha + P\hat{H}Q\gamma$$
$$i\dot{\gamma} = Q\hat{H}P\alpha + Q\hat{H}Q\gamma$$

Applying the principle of adiabatic elimination, i.e. $\dot{\gamma} \to 0$, we obtain an equation of

motion for the low energy part only

$$i\dot{\alpha} = \left(P\hat{H}P - P\hat{H}Q\frac{1}{Q\hat{H}Q}Q\hat{H}P \right) \alpha$$

This can be expressed in terms of an effective Hamiltonian for the low-energy subspace:

$$\hat{H}_{\text{eff}} \approx P\hat{H}P - P\hat{H}Q\frac{1}{Q\hat{H}Q}Q\hat{H}P \tag{2.12}$$

This method is widely used, for example, in condensed matter and quantum optics to derive effective low-energy theories by eliminating virtual transitions to excited states, and it can be applied to systematically obtain effective models for qubits embedded in higher-dimensional Hilbert spaces by projecting out non-computational (excited) states.

Exercises

Exercise 2.1 ***Changing bases***

Consider a general two-body state

$$|\psi\rangle = a\,|00\rangle + b\,|01\rangle + c\,|10\rangle + d\,|11\rangle$$

- *Express the state $|\psi\rangle$ in the $|+\rangle, |-\rangle$ basis, where $|+\rangle$ and $|-\rangle$ are eigenstates of the Pauli X operator:*

$$\hat{\sigma}_x\,|+\rangle = |+\rangle \qquad \hat{\sigma}_x\,|-\rangle = -\,|-\rangle$$

- *Under which conditions will the form of the state remain unchanged when expressed in the $|+\rangle, |-\rangle$ basis? Determine if the corresponding state is entangled.*

Exercise 2.2 ***Hermitian operators have real eigenvalues***

Consider the Pauli operator σ_y:

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

1. *Show that σ_y is a Hermitian operator.*

$$\sigma_y^\dagger = \sigma_y$$

2. *Calculate the eigenvalues of σ_y.*
3. *Prove that for any Hermitian operator $\hat{A}$, if $|\psi\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue λ, then λ must be real.*
4. *Using this result to explain why energy measurements in quantum mechanics always yield real values.*

Exercise 2.3 ***Measurements***

Suppose that the state of the system is

$$|\psi\rangle = \sum_j a_j |\phi_j\rangle$$

where $|\phi_j\rangle$ are eigenstates of a physical observable $\hat{A}$, i.e.

$$\hat{A}|\phi_j\rangle = \lambda_j|\phi_j\rangle.$$

Suppose a measurement of the observable $\hat{A}$ is performed. What are the possible outcomes, their probabilities, and the post-measurement state of the system?

Exercise 2.4 *Bloch vector representation*

Consider two one-qubit states $|\phi\rangle$ and $|\chi\rangle$ that are orthogonal, meaning their inner product is zero:

$$\langle\phi|\chi\rangle = 0$$

Recall that any pure one-qubit state can be represented as a point on the Bloch sphere, with the corresponding Bloch vector $\vec{r} = (x, y, z)$ satisfying $|\vec{r}| = 1$.

1. *Express the inner product of two arbitrary one-qubit states in terms of their Bloch vectors $\vec{r}_\phi$ and $\vec{r}_\chi$.*
2. *Given that $\langle\phi|\chi\rangle = 0$, what is the relationship between their corresponding Bloch vectors $\vec{r}_\phi$ and $\vec{r}_\chi$?*
3. *Calculate the inner product of the Bloch vectors $\vec{r}_\phi \cdot \vec{r}_\chi$.*
4. *Explain the geometric interpretation of your result in terms of the Bloch sphere representation.*

Exercise 2.5 *Properties of the density operator*

*Which of these operators are **not** valid physical density operators?*

1. $|+\rangle\langle+|$, *where* $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$
2. $\frac{1}{2}|0\rangle\langle 0| - \frac{1}{2}|0\rangle\langle 1| + \frac{1}{2}|1\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$
3. $\frac{1}{3}|0\rangle\langle 0| + \frac{2}{3}|1\rangle\langle 1|$
4. $\frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| + \frac{i}{4}(|0\rangle\langle 1| + |1\rangle\langle 0|)$
5. $\frac{1}{2}\mathbb{1} + \frac{1}{2}\sigma_z$, *where* $\mathbb{1}$ *is the identity matrix and* σ_z *is the Pauli Z matrix*

Exercise 2.6 *Expectation values*

Show that the expectation value of a general observable $\hat{A}$ can be written $Tr(\hat{\rho}\hat{A})$