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I Information, Entropy, and Computational Complexity

1. Information is a Physical Entity

1.1 Quantifying Information

If X is a random variable over a set of events x such that event x occurs with probability p_x , then the **Shannon entropy** of event x is $-\log_2(p_x)$.

1.2 A Thermodynamics Problem

That is to say, if there are M different positions to locate a molecule in the final state, there are only $p_1 M$ positions for it in the initial state.

1.3 Information is Physical

If we consider a set of possible events whose probabilities of occurrence are p_1, p_2, \dots, p_n , the average information is

$$H = \langle I(p_i) \rangle \sim - \sum_{i=0}^n p_i \log_2 p_i$$

Erasure is irreversible! To erase, we must dissipate heat in the surroundings. The entropy of the surroundings must go up by at least $k_B \ln 2$. This result, which demonstrates the intimate link between thermodynamics and information theory, has been verified experimentally. (信息的擦除会产生热量, 这是信息与热力学的联系)

1.4 Data Compression

In general, we model a set of data to be compressed by a random variable X . The Shannon entropy of X is then defined as the expected logarithm of the probability:

$$H(X) = - \sum_x P(X = x) \log_2 P(X = x)$$

The probability of finding a sequence X_1, X_2, \dots, X_n is

$$P(X_1, X_2, \dots, X_n) = \prod_i P(X_i) \approx \prod_x P(X = x)^{nP(X=x)}$$

The information content is approximately

$$P(X_1, X_2, \dots, X_n) = 2^{-nH(X)}$$

This shows that there are at most 2^{nH} typical sequences, and, hence, it only requires $nH(X)$ bits to encode them.

2. Computational Complexity

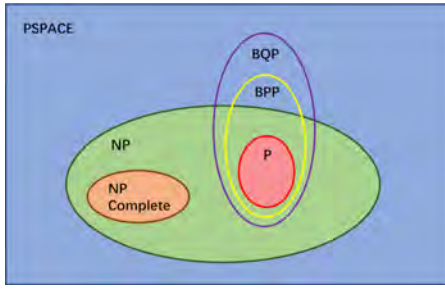


Figure 1: Problems

- 1) Information and Physics
- 2) Computational Complexity

2.1 Decision Problems: P vs NP

Most computational problems can be formulated as decision problems, whose answer is yes or no.

- P class: Problems can be solved by Polynomial time algorithm.
- NP class: Problems for which a solution can be checked in Polynomial time.
- NP -Complete Problem: If any of these problems can be solved by polynomial worst-case time algorithm, then all can be solved by polynomial worst-case time algorithms.

2.2 Randomness

A problem is in BPP (bounded-error probabilistic polynomial time) if there is an algorithm for it that has the following properties:

- It is allowed to flip coins and make random decisions.
- It is guaranteed to run in polynomial time.
- On any given run of the algorithm, it has a probability of at most $1/3$ of giving the wrong answer, whether the answer is YES or NO.

Strong Church-Turing Thesis: Any model of computation can be simulated on a probabilistic Turing machine with at most a polynomial increase in the number of elementary operations required.

2.3 Quantum Randomness

A quantum information processor differs from a classical one (a Turing machine) in two important ways:

- 1) The input can be prepared not only in the binary form, but also in any superposition state.
- 2) Intervention (such as examine the state of the machine) could modify the state of the quantum machine, and it would not be possible to resume the processing operation.

In many ways, quantum mechanics generalizes real probability to complex probability amplitudes. One can generalize the classical BPP class to BQP .

[quantumalgorithmzoo](#) (or, [quantum-algorithm-zoo](#) in Chinese).

3. Quantum Computing Milestones

1994 Peter Shor's algorithm for factoring integers ignited a tremendous increase of interest in quantum computing.

2018 Google declared quantum supremacy, the potential ability of quantum computing devices to solve problems that classical computers practically cannot.

2019 IBM launched first 20-qubit commercial quantum computer named Q System One. Organizations started to prepare for the second quantum revolution by education in quantum engineering.

II Photons and Their Quantum States in a Complex Vector Space

From Numbers to Complex Vectors

In classical computing, there are $\mathbb{N} \subset \mathbb{Z} \subset \mathbb{Q} \subset \mathbb{R} \subset \mathbb{C}$.

Let K be a field (域), which is a set (e.g., \mathbb{R} or \mathbb{C}) where ordinary addition, subtraction, multiplication and division are well-defined. A **vector space** V is a set where the addition of two vectors and a multiplication by an element of K , so-called a scalar, are defined.

An element of $V = \mathbb{C}_n$ can be expressed as a column of n complex numbers $\chi_i (1 \leq i \leq n)$ as

$$|x\rangle = \begin{pmatrix} \chi_1 \\ \vdots \\ \chi_n \end{pmatrix}, \chi_i \in \mathbb{C}$$

1. Photon Polarization, an Example

The polarization of a photon is an example of a two-dimensional complex vector space (i.e., a qubit). we can use a complex vector to represent an arbitrary polarization. The polarization of a photon can be measured by an analyzer, which allows the photon to pass with a probability.

1.1 The Polarization of Light

Property I Light is an electromagnetic wave. It is transverse, which means that the electric (and magnetic) field of a light wave is perpendicular to the propagation direction.

Recall that a planar and monochromatic scalar wave traveling in the z direction has an amplitude of vibration

$$u(z, t) = u_0 \cos(kz - \omega t)$$

where the speed of the wave $c = \frac{\omega}{k}$.

At $z = 0$ (which can be generalized for arbitrary z),

$$u(t) \equiv u(z = 0, t) = u_0 \cos \omega t$$

For an electromagnetic wave, what oscillates is an E vector in the $x - y$ plane (we ignore B for simplicity).

Property II Light waves (with vector nature of \vec{E}) can be decomposed into two rays by birefringent crystals, such as Iceland spar.

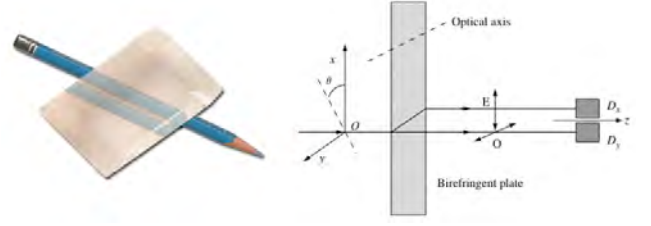


Figure 2: Property II

For light with linear polarization

$$E_x = E_0 \cos \theta \cos \omega t$$

$$E_y = E_0 \sin \theta \cos \omega t$$

So we can write

$$\vec{E} = E_0 \hat{p} \cos \omega t, \hat{p} = (\cos \theta, \sin \theta)$$

This can be achieved by letting light pass through a polarizer whose axis makes an angle θ with x axis. The intensity of the light is proportional to the square electric field $I \propto E_0^2$.

The Malus law $I' = I \cos^2 \theta$.

In general, we have elliptical polarization

$$E_x = E_0 \cos \theta \cos(\omega t - \delta_x) = E_0 \operatorname{Re}(\mu e^{-i\omega t})$$

$$E_y = E_0 \sin \theta \cos(\omega t - \delta_y) = E_0 \operatorname{Re}(\nu e^{-i\omega t})$$

where $\mu = \cos \theta e^{i\delta_x}$ and $\nu = \sin \theta e^{i\delta_y}$, so $|\mu|^2 + |\nu|^2 = 1$. It is important to note that only $\delta = \delta_y - \delta_x$ is physically relevant. This is because, by a time shift, we can choose $\delta_x = 0$.

Therefore, we can use a complex vector $\begin{pmatrix} \mu \\ \nu \end{pmatrix}$ to represent an arbitrary polarization. The polarization vector is the same as $\begin{pmatrix} \mu e^{i\phi} \\ \nu e^{i\phi} \end{pmatrix}$ for arbitrary ϕ .

1.2 The Quantum Interpretation

Light is composed of photons, or light quanta. The Malus law now has a statistical interpretation, as photons cannot be further divided.

2. Dirac's Bracket Notation

A complex vector space is composed of elements $|a\rangle$ called **kets**. They are column vectors in our usual notation. It has a dual space whose elements are **bras** $\langle a|$. **Inner**

product $\langle a|b\rangle$ generalizes the dot product of usual vectors. Notice $\langle a|b\rangle = \langle b|a\rangle^\dagger$. Choosing an **orthonormal basis** of kets $|i\rangle$ (notice $\langle i|j\rangle = \delta_{ij}$), we can expand an arbitrary ket $|a\rangle$ as

$$|a\rangle = \sum_i |i\rangle \langle i|a\rangle$$

2.1 Vector Space in Quantum Mechanics

In quantum mechanics, a vector space is composed of elements $|a\rangle$, known as **kets** or ket-vectors (following Dirac's invention). It satisfies the following axioms.

- 1) The sum of any two kets is also a ket:
- 2) Vector addition is commutative:
- 3) Vector addition is associative:
- 4) There is a unique vector 0 such that when you add it to any ket, it gives the same ket back:

$$|a\rangle + 0 = |a\rangle$$

- 5) Given any ket $|a\rangle$, there is a unique $-|a\rangle$ such that:

$$|a\rangle + (-|a\rangle) = 0$$

The following two axioms involves the multiplication by any complex number. Ordinary vectors, however, can only be multiplied by real numbers.

- (6) Given any ket $|a\rangle$ and any complex number ζ , you can multiply them to get a new ket. Also multiplication by a scalar is linear:

$$|a'\rangle = |\zeta a\rangle = \zeta |a\rangle$$

- (7) The distributive property holds:

$$\begin{aligned} \zeta(|a\rangle + |b\rangle) &= \zeta |a\rangle + \zeta |b\rangle \\ (\zeta + \omega) |a\rangle &= \zeta |a\rangle + \omega |a\rangle \end{aligned}$$

2.2 The Complex Conjugate Vector Space

A complex vector space has a dual space, i.e., the complex conjugate vector space.

For every ket $|a\rangle$, there is a **bra** or bra-vector $\langle a|$ in the dual space. Bras satisfy the same axiom as kets, with two notable differences:

- Suppose $\langle a|$ and $\langle b|$ are the bras corresponding to the kets $|a\rangle$ and $|b\rangle$, respectively. Then the bra corresponding to $|a\rangle + |b\rangle$ is:

$$\langle a| + \langle b|$$

- The bra corresponding to $\zeta |a\rangle$ for any complex number ζ is

$$(\zeta |a\rangle)^\dagger = \langle a| \zeta^\dagger = \zeta^\dagger \langle a|$$

2.3 Inner Products

The analog to the dot product for ordinary vectors is the **inner product** for a bra and a ket is $\langle b|a\rangle$, which is a complex number.

- The inner products are linear:
- Interchanging bras and kets corresponds to complex conjugation:

$$\langle b|a\rangle = \langle a|b\rangle^\dagger$$

Hence, $\langle a|a\rangle$ is a real number.

For example, if ket $|a\rangle$ and $|b\rangle$ are represented by the column vectors

$$|a\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{pmatrix}, |b\rangle = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \end{pmatrix}$$

then the corresponding bra $\langle b|$ is represented by the row vector

$$\langle b| = (\beta_1^\dagger \quad \beta_2^\dagger \quad \beta_3^\dagger \quad \beta_4^\dagger \quad \beta_5^\dagger)$$

The inner product is defined as the product of the row vector and column vector:

$$\begin{aligned} \langle b|a\rangle &= (\beta_1^\dagger \quad \beta_2^\dagger \quad \beta_3^\dagger \quad \beta_4^\dagger \quad \beta_5^\dagger) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{pmatrix} \\ &= \beta_1^\dagger \alpha_1 + \beta_2^\dagger \alpha_2 + \beta_3^\dagger \alpha_3 + \beta_4^\dagger \alpha_4 + \beta_5^\dagger \alpha_5 \end{aligned}$$

Observe that $\langle b|a\rangle = \langle a|b\rangle^\dagger$

2.4 Normalized and Orthogonal Vectors

Normalized vector is a generalization of unit vector in ordinary space. Normalized vectors satisfy

$$\langle a|a\rangle = 1$$

In ordinary space, vectors are orthogonal if their dot product is zero (they are also said to be perpendicular to each other). In Hilbert space, two vectors are orthogonal if

$$\langle b|a\rangle = 0$$

2.5 Basis and Basis Vectors

Let us consider a set of k vectors $\{|x_1\rangle, \dots, |x_k\rangle\}$ in $V = \mathbb{C}_n$. The set is said to be linearly dependent if the equation

$$\sum_{i=1}^k \eta_i |x_i\rangle = |0\rangle$$

has a solution η_1, \dots, η_k , at least one of which is non-vanishing.

If the trivial solution $\eta_i = 0 (1 \leq i \leq k)$ is the only solution, the set is said to be **linearly independent**.

The set of n linearly independent vectors is called a **basis** of \mathbb{C}_n and the vectors are called **basis vectors**.

2.6 Orthonormal Basis and Completeness

Any vector $|a\rangle$ can be written as a sum of basis

$$|a\rangle = \sum_i \alpha_i |i\rangle$$

where the complex number α_i are called the components of the vector.

We can calculate an individual component corresponding to the basis vector $|j\rangle$ as

$$\alpha_j = \langle j|a\rangle$$

since $\langle j|i\rangle = \delta_{ij}$ (i.e. 1 if $i = j$ else 0).

Therefore, we can also rewrite the decomposition of the vector $|a\rangle$ in a more elegant form as

$$|a\rangle = \sum_i |i\rangle \langle i|a\rangle$$

which implies the following identity:

$$\sum_i |i\rangle \langle i| = I$$

where I is an identity operator $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ (note that we will come back to the definition of operator).

2.7 Projection Operators

The matrix

$$P_k = |k\rangle \langle k|$$

introduced above is called a **projection operator** (投影算符) in the direction defined by $|k\rangle$. This projects a vector $|v\rangle$ to a vector parallel to $|k\rangle$ in such a way that $|v\rangle - P_k |v\rangle$ is orthogonal to $|k\rangle$.

The set $\{P_k = |k\rangle \langle k|\}$ satisfies the conditions

- 1) $P_k^2 = P_k$
- 2) $P_k P_j = 0 (k \neq j)$
- 3) $\sum_k P_k = I$ (completeness relation)

3. Photon Polarization in the New Language

Photon polarization lives in a 2D complex vector space. An orthonormal basis can be chosen to be linear polarization along x and y axes.

$$|h\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |v\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The corresponding projection operators are

$$P_h = |h\rangle \langle h| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, P_v = |v\rangle \langle v| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

We confirm the completeness condition $P_h + P_v = I_{2 \times 2}$

A general state $|p\rangle$ of a photon is represented by a unit vector

$$|p\rangle = I |p\rangle = |h\rangle \langle h|p\rangle + |v\rangle \langle v|p\rangle = \mu |h\rangle + \nu |v\rangle$$

where $\mu, \nu \in \mathbb{C}$ and $\langle p|p\rangle = |\mu|^2 + |\nu|^2 = 1$

The components of $|p\rangle$,

$$\mu = \langle h|p\rangle, \nu = \langle v|p\rangle$$

are known as the **probability amplitudes**.

The probabilities for the measurements of horizontal and vertical polarizations are given by

$$P_h = |\mu|^2 = \langle p|h\rangle \langle h|p\rangle \equiv \langle p|P_h|p\rangle$$

$$P_v = |\nu|^2 = \langle p|v\rangle \langle v|p\rangle \equiv \langle p|P_v|p\rangle$$

The total probability $P_h + P_v = 1$. After the measurement, the photon is either in the state $|h\rangle$ or in the state $|v\rangle$.

III Spins, Qubits and Linear Operators

In the quantum world, state and measurement are two different things.

1. The Stern-Gerlach Experiment

In the Stern-Gerlach experiment, a narrow beam of silver atoms passes through an electromagnet [with a nonuniform $\vec{B}(z) = B(z)\hat{z}$] and then lands on a glass detector plate.

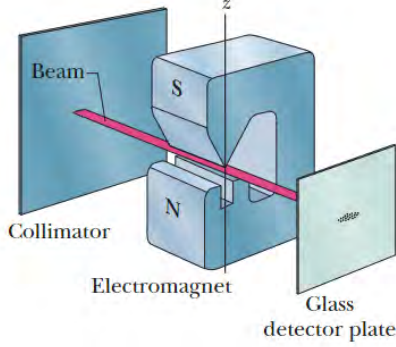


Figure 3: The Stern-Gerlach Experiment

In fact, spin states also belong to the 2D complex vector space \mathbb{C}^2 .

2. Spin, Qubit, and the Bloch Sphere

The isolated quantum spin ($S = 1/2$) is our second realization of the general class of two-level systems which we call **qubits**, or quantum bits.

A classical computer operates on strings of zeros and ones, such as 1001001001. Each position in such a string is called a (classical) bit, and it contains either a 0 or a 1. The abstract bit can be represented by a physical system.

We can take the two states of a classical bit to be represented by two orthogonal unit vectors in a two-dimensional space,

$$|0\rangle \equiv |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle \equiv |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Classically, we either have state $|0\rangle$, or state $|1\rangle$, but not both simultaneously.

In quantum mechanics, however, the two states can be superimposed, i.e., we promote the states of a classical bit to be two basis vectors in \mathbb{C}^2 .

As we know, a general state of a qubit is

$$|\phi\rangle = \alpha |0\rangle + \beta |1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \alpha, \beta \in \mathbb{C}$$

normalized by (the probabilistic interpretation)

$$\langle\phi|\phi\rangle = |\alpha|^2 + |\beta|^2 = 1$$

We can parametrize it, alternatively, by

$$|\phi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$$

and represented it by a point on the **Bloch sphere**.

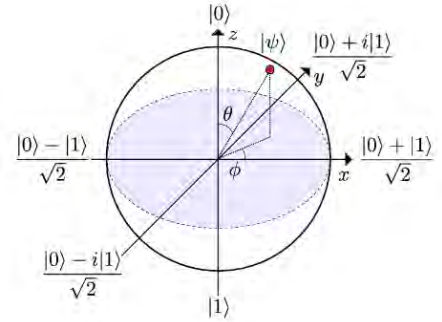


Figure 4: The Bloch sphere

3. Linear Operators and Matrices

3.1 Measuring a Quantum Spin

Knowing a quantum state, on the other hand, means knowing as much as can be known about how the system was prepared. Perhaps the most difficult things to accept is that quantum mechanics is unavoidably unpredictable. It is a complete calculus of probabilities.

At the center of the calculus is the idea of an observable or a measurable, i.e., a property one can measure with a proper apparatus.

3.2 Linear Operators

We will introduce an axiom: physical observables are described by linear operators.

A map $M : \mathbb{C}^n \rightarrow \mathbb{C}^n$ is a **linear operator** if

$$M(\mu|x\rangle + \nu|y\rangle) = \mu M|x\rangle + \nu M|y\rangle$$

is satisfied for arbitrary $|x\rangle, |y\rangle \in \mathbb{C}^n$ and $\mu, \nu \in \mathbb{C}$.

The definition expresses the following facts.

1) M acts on a vector $|a\rangle$ to give $|b\rangle$ in the same space of states:

$$M|a\rangle = |b\rangle$$

2) When M acts on a multiple of an input vector, it gives the same multiple of the output vector:

$$M\zeta|a\rangle = \zeta|b\rangle.$$

3) When M acts on a sum of vectors, the results are simply the sum of the output vectors:

$$M\{|a\rangle + |b\rangle\} = M|a\rangle + M|b\rangle.$$

3.3 Matrix Representation of Linear Operators

Given the choice of basis vectors, bra and ket vectors are represented by row and column vectors. If the vector space is N -dimensional, we can choose a set of N orthonormal ket-vectors $|j\rangle$ and their dual bra-vectors $\langle j|$.

In component form, we can write

$$|a\rangle = \sum_{j=1}^N \alpha_j |j\rangle, \quad |b\rangle = \sum_{j=1}^N \beta_j |j\rangle$$

Plugging the substitutions into $M|a\rangle = |b\rangle$, we obtain

$$\sum_{j=1}^N M|j\rangle \alpha_j = \sum_{j=1}^N \beta_j |j\rangle$$

The inner product of both sides with a particular basis vector $\langle k|$ gives

$$\sum_{j=1}^N \langle k|M|j\rangle \alpha_j = \sum_{j=1}^N \beta_j \langle k|j\rangle = \beta_k$$

where the second identity is obtained because $\langle k|j\rangle = \delta_{kj}$.

Symbolically, we can define an $N \times N$ matrix

$$M = \begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1N} \\ m_{21} & m_{22} & \cdots & m_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ m_{N1} & m_{N2} & \cdots & m_{NN} \end{pmatrix}$$

where $m_{kj} \equiv \langle k|M|j\rangle$ are called matrix elements.

The inner product of $M|a\rangle = |b\rangle$ with $\langle k|$ becomes

$$\sum_j m_{kj} \alpha_j = \beta_k$$

for $k = 1, 2, \dots, N$.

One recognizes that this is nothing but the matrix multiplication

$$\begin{pmatrix} m_{11} & m_{12} & \cdots & m_{1N} \\ m_{21} & m_{22} & \cdots & m_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ m_{N1} & m_{N2} & \cdots & m_{NN} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_N \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_N \end{pmatrix}$$

which can simply be abbreviated as $M|a\rangle = |b\rangle$, in which M , $|a\rangle$, $|b\rangle$ are now represented by the matrix and two vectors.

3.4 Eigenvalues and Eigenvectors

For the application of a linear operator on a vector, such as $M|a\rangle = |b\rangle$, we do not expect, in general, $|b\rangle = \alpha|a\rangle$, where $\alpha \in \mathbb{C}$.

However, along certain directions, we find ket-vectors $|\lambda\rangle$ such that

$$M|\lambda\rangle = \lambda|\lambda\rangle,$$

where λ are called **eigenvalues**, while $|\lambda\rangle$ the corresponding **eigenvectors**.

In general, eigenvalues are complex numbers. For example,

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

However, observable quantities in quantum mechanics are represented by Hermitian operators, i.e., linear operators that are equal to their own Hermitian conjugate ($M^\dagger = \overline{M^T}$, 转置复共轭).

- If $M|a\rangle = |b\rangle$, then $\langle a|M^\dagger = \langle b|$ in general. For Hermitian M , we further have $\langle a|M = \langle b|$.

- It follows that the eigenvalues of a Hermitian matrix are real.

According to mathematics, the eigenvectors of a Hermitian operator form an orthonormal basis—this serves as a foundation of quantum mechanics.

- The eigenvectors of a Hermitian operator are a complete set, i.e. any vector the operator can generate can be expanded as a sum of its eigenvectors.

- If λ_1 and λ_2 are two unequal eigenvalues of a Hermitian operator, then the corresponding eigenvectors are orthogonal.

- Even if the two eigenvalues are equal (i.e., degenerate), the corresponding eigenvectors can be chosen to be orthogonal.

Therefore, we often replace an operator by its spectral decomposition (note we insert two identity operators)

$$M = \sum_{\lambda\lambda'} |\lambda\rangle \langle\lambda|M|\lambda'\rangle \langle\lambda'| = \sum_{\lambda} \lambda |\lambda\rangle \langle\lambda| = \sum_{\lambda} \lambda P_{\lambda}$$

4. The Principles of Quantum Mechanics

States of a system are represented by vectors in a complex vector space.

- 1) The observables or measurable quantities of quantum mechanics are represented by linear operators L .
- 2) The possible results of a measurement are the eigenvalues λ of the operator that represents the observable.
- 3) Unambiguously distinguishable states are represented by orthogonal vectors.
- 4) If $|\phi\rangle$ is a state-vector, and the observable L is measured, the probability to observe λ is $P_{\lambda} = \langle\phi|\lambda\rangle \langle\lambda|\phi\rangle$, where $|\lambda\rangle$ is the corresponding eigenvector.

4.1 Constructing Spin Operators

Principle 1 states that each component of spin (denoted by σ) is represented by a linear operator. We begin with σ_z along the z direction.

Principle 2 states that σ_z has two eigenvalues ± 1 with corresponding eigenvectors, i.e.,

$$\sigma_z |0\rangle = |0\rangle, \sigma_z |1\rangle = -|1\rangle$$

Principle 3 emphasizes that $\langle 0|1\rangle = 0$. Therefore, as we learned above, the matrix representation of σ_z is

$$\sigma_z = \begin{pmatrix} \langle 0|\sigma_z|0\rangle & \langle 0|\sigma_z|1\rangle \\ \langle 1|\sigma_z|0\rangle & \langle 1|\sigma_z|1\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where we also use $\langle 0|0\rangle = \langle 1|1\rangle = 1$.

Principle 4 states that for a spin in $|\phi\rangle = \alpha |0\rangle + \beta |1\rangle$, $|\alpha|^2 = \alpha * \alpha$ is the probability of the spin being up, or that the spin would be measured as $\sigma_z = +1$. Likewise, $|\beta|^2 = \beta * \beta$ is the probability of the spin being down, or that the spin would be measured as $\sigma_z = -1$.

To construct σ_x and σ_y ,

We can also rotate the apparatus to align along x axis and measure the spin component to be either $+1$ or -1 . This means that we can define two basis states by

$$\sigma_x |r\rangle = |r\rangle, \sigma_x |l\rangle = -|l\rangle$$

Thus, we need to know, e.g., what α and β are, such that

$$|r\rangle = \alpha |0\rangle + \beta |1\rangle$$

In physics, we determine them by experimental measurements, not mathematical axioms.

Therefore, experiments tell us that

$$|r\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{e^{i\phi}}{\sqrt{2}} |1\rangle$$

There is some ambiguity in choosing the phase ϕ , but it is nothing more than the ambiguity in our choice of the exact direction for the x axis. We can simply choose $\phi = 0$, so

$$|r\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$$

Using $\langle r|l\rangle = 0$ and $\langle l|l\rangle = 1$, we find

$$|l\rangle = \frac{1}{\sqrt{2}} |0\rangle - \frac{1}{\sqrt{2}} |1\rangle$$

There can be an overall phase factor in $|r\rangle$ and $|l\rangle$, but it is not measurable.

The matrix representation of σ_x must, then, satisfy

$$\begin{pmatrix} (\sigma_x)_{00} & (\sigma_x)_{01} \\ (\sigma_x)_{10} & (\sigma_x)_{11} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} (\sigma_x)_{00} & (\sigma_x)_{01} \\ (\sigma_x)_{10} & (\sigma_x)_{11} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = - \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

The solution to the two matrix equations is

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

In a similar, but more complicated way, we can obtain

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

whose eigenvectors, with eigenvalues ± 1 , are

$$|i\rangle = \frac{1}{\sqrt{2}} |0\rangle + \frac{i}{\sqrt{2}} |1\rangle, |o\rangle = \frac{1}{\sqrt{2}} |0\rangle - \frac{i}{\sqrt{2}} |1\rangle$$

4.2 Along an Arbitrary Direction

The three spin operators, represented by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are known as **Pauli matrices**. It is tempting to write

$$\vec{\sigma} = \sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}$$

This is correct. In fact, spin is a 3-vector operator.

It is good time to distinguish the two notions of vectors.

- We live in a 3D world. Spin, like displacement and momentum, is a 3-vector. It has operator (not scalar) components along the three spatial directions.
- The quantum state of a spin is a state-vector in a 2D complex vector spaces (of spin states).

Therefore, the relevant operator for measuring the spin along an arbitrary direction $\hat{n} = (n_x, n_y, n_z)$ is

$$\begin{aligned} \sigma_n &= \vec{\sigma} \cdot \hat{n} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z \\ &= \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix} \end{aligned}$$

One can check that the eigenvalues, or the measurement results, are, again, ± 1 .

$$\sigma_z = |0\rangle\langle 0| - |1\rangle\langle 1|$$

4.3 Irreversibility of Measurement

Measurement is like blocking one of the paths. Along the other path, you either get the particle, or you do not. You do not know when you get it, but you know the probability of getting it.

Quantum measurement is an irreversible operation. After the measurement, the system is in one of the eigenstates. The pre-measurement state collapses or reduces to the post-measurement state, as a consequence of the measurement (the Copenhagen interpretation).

We emphasize that when an operator acts on a state-vector, it produces a new state-vector in general. The new vector has nothing to do with the post-measurement state, although we can use it to calculate the average or

expectation value of the measurable quantit (退相干丢失了信息).

L. Susskind and A. Friedman, Quantum Mechanics (Basic Books, 2014), Chaps. 3-4.

IV Quantum Entanglement

1. Multiple Qubits and Tensor Products

1.1 Tensor Products

A pair of classical bits can have (or be in) any of the four possible states 00, 01, 10, 11.

If a bit is represented by $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, the two-bit states can be represented by four column vectors

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

They are examples of tensor products.

In general, the **tensor product** of an $m \times n$ matrix (vector) A and a $p \times q$ matrix (vector) B is an $mp \times nq$ matrix in the form

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix}$$

The tensor product of two vectors $|u\rangle$ and $|v\rangle$ is often abbreviated as $|u\rangle|v\rangle$ or $|uv\rangle$, as was done above.

$$\sigma_{1x} = \sigma_x \otimes I, \sigma_{1y} = \sigma_y \otimes I, \sigma_{1z} = \sigma_z \otimes I$$

$$\sigma_{2x} = I \otimes \sigma_x, \sigma_{2y} = I \otimes \sigma_y, \sigma_{2z} = I \otimes \sigma_z$$

2. Entangled States and EPR Paradox

2.1 Combining Two Qubits

In the case of two qubits the vector space is, therefore, four-dimensional, with an orthonormal basis

$$|00\rangle, |01\rangle, |10\rangle, |11\rangle$$

The general state $|\Psi\rangle$ that nature allows us to associate with two qubits is any normalized superposition of the four orthogonal classical states,

$$|\Psi\rangle = \alpha_1 |00\rangle + \alpha_2 |01\rangle + \alpha_3 |10\rangle + \alpha_4 |11\rangle$$

with the complex amplitudes being constrained only by the normalization condition 1.

In other words, two-qubit states are unit vectors in $(\mathbb{C}^2)^{\otimes 2} = \mathbb{C}^2 \otimes \mathbb{C}^2$.

- If the first qubit is in $\alpha_1 |0\rangle + \beta_1 |1\rangle$, and the second qubit is in $\alpha_2 |0\rangle + \beta_2 |1\rangle$, then the **product state** is

$$\begin{aligned} & (\alpha_1 |0\rangle + \beta_1 |1\rangle) \otimes (\alpha_2 |0\rangle + \beta_2 |1\rangle) \\ &= \alpha_1 \alpha_2 |00\rangle + \alpha_1 \beta_2 |01\rangle + \beta_1 \alpha_2 |10\rangle + \beta_1 \beta_2 |11\rangle \end{aligned}$$

- In the two case, even though we put the two qubits together, the information they encode is still separable. If we operate on the first qubit only, the second remains unchanged:

$$(L \otimes I)(|u\rangle \otimes |v\rangle) = (L|u\rangle) \otimes |v\rangle$$

It takes 4 real parameters to specify a two-qubit product state (or separable state). But, it takes 6 real parameters to specify the most general two-qubit state.

Obviously, the space of all two-qubit states is much richer than that of the product states, which can be prepared separately for each qubit.

The other class of states are known as the **entangled states**, exemplified by the famous Bell states. One of the four Bell states is

$$|\Psi_+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

In the state particle 1 can be in state $|0\rangle$ and particle 2 in state $|1\rangle$, or vice versa, but there is no way of knowing which particle is in which state. All that is defined is the fact that the two qubits are different.

2.2 EPR Paradox

Entanglement is closely linked to the issue of locality (or non-locality) in quantum theory. In particular, if the two particles in an entangled state are widely separated, then a measurement on one will immediately influence the quantum state of the other one. It seems as if the particles are communicating faster than the speed of light.

In Bohm's version of the EPR paradox, the two particles are in the Bell state

$$|\Psi_+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

One can measure the first qubit according to the following measurement rule

$$|\Psi\rangle = \begin{pmatrix} \alpha_0 |0\rangle |\Phi_0\rangle \\ + \alpha_1 |1\rangle |\Phi_1\rangle \end{pmatrix} \xrightarrow{\text{M}} \begin{matrix} |x\rangle \\ |\Phi_x\rangle \end{matrix} \quad p = |\alpha_x|^2$$

Upon the measurement of particle 1, one knows the state of the faraway particle 2 instantaneously. Indeed, modern experiments have confirmed that their properties remain entangled after they are sent far apart.

However, the special theory of relativity is not violated because no information travels faster than light (local in the quantum field theoretical sense). Before the measurement, particle 2 has equal probabilities in states $|0\rangle$ and $|1\rangle$. This remains to be true (in terms of an external observer's statistical model) after the measurement. The measurement of particle 1 does not a priori fix the state of particle 2; there is no information transfer. (其实信息传递并无超光速, 即纠缠虽然状态相反, 但并未传递信息, 信息是在之前就传到了)

2.3 Information in the Bell State

The two-particle Bell state cannot be written as the tensor product of single-particle states. The single-particle states are entangled, not separable, in such superpositions. This means that all of the information is distributed among two qubits (i.e., not local), and that none of the individual systems carries any information. This is the essence of entanglement and is one of the novel and counterintuitive features of quantum mechanics. For further illustration, we introduce the concept of expectation values, or average values.

Suppose we consider an experiment that measures an observable L , whose eigenvalues are λ with corresponding eigenvectors $|\lambda\rangle$, i.e., $L|\lambda\rangle = \lambda|\lambda\rangle$.

Suppose that the normalized state of a quantum system is ψ , which can be expanded in the orthonormal basis $\{|\lambda\rangle\}$:

$$|\psi\rangle = \sum_{\lambda} |\lambda\rangle \langle\lambda|\psi\rangle$$

Let L operate on ψ :

$$L|\psi\rangle = \sum_{\lambda} L|\lambda\rangle \langle\lambda|\psi\rangle = \sum_{\lambda} \lambda|\lambda\rangle \langle\lambda|\psi\rangle$$

The **expectation value** (期待值) of L of the system is defined as

$$\langle L \rangle \equiv \langle\psi|L|\psi\rangle = \sum_{\lambda} \lambda \langle\psi|\lambda\rangle \langle\lambda|\psi\rangle = \sum_{\lambda} \lambda P(\lambda)$$

This is the weighted sum of L 's eigenvalues λ with probability $P(\lambda) = \langle\psi|\lambda\rangle \langle\lambda|\psi\rangle$.

Suppose we perform a large number of identical experiments. We can identify $P(\lambda)$ as the percentage of observations whose result is λ . In the statistical sense, the experimental average is identical to the mathematical definition of $\langle L \rangle$.

For a one-qubit state $|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\phi} \sin \frac{\theta}{2} |1\rangle$ one can always find a particular direction \hat{n} for which $\langle \vec{\sigma} \cdot \hat{n} \rangle = 1$. One can check $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ is the direction. This still holds when we measure one of the qubit in a two-qubit product state, such as $|\psi\rangle \otimes |\psi'\rangle$.

However, if one measures the first qubit in the Bell state $|\Psi_+\rangle$, the result is $\langle \vec{\sigma}^{(1)} \cdot \hat{n} \rangle = 0$ for any \hat{n} . Let us operate $\sigma_n^{(1)} = \vec{\sigma}^{(1)} \cdot \hat{n}$, or more precisely 1:

$$\begin{aligned} \sigma_n^{(1)} |\Psi_+\rangle &\propto (\cos \theta |0\rangle + e^{i\phi} \sin \theta |1\rangle) |1\rangle \\ &\quad + (e^{-i\phi} \sin \theta |0\rangle - \cos \theta |1\rangle) |0\rangle \end{aligned}$$

A quick comparison with $|\Psi_+\rangle \propto |01\rangle + |10\rangle$ shows that

$$\langle \Psi_+ | \vec{\sigma}^{(1)} \cdot \hat{n} | \Psi_+ \rangle = 0$$

regardless of the direction of \hat{n} .

If the expectation value of a component of $\vec{\sigma}^{(1)}$ vanishes, it means that the experimental outcome is equally likely to be ± 1 . In other words, the outcome is completely uncertain. Assume Charlie prepare two qubits in the entangled state and send one qubit to Alice and one to Bob without looking at (i.e., measuring) the qubits. Although Alice and Bob know exactly what the combined system is in, they can predict nothing about the outcome of their individual measurements.

We have constructed the dot product of the vector-operator $\vec{\sigma}^{(1)}$ and $\vec{\sigma}^{(2)}$, which is manifestly rotational invariant,

$$\vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} = \sigma_x^{(1)} \sigma_x^{(2)} + \sigma_y^{(1)} \sigma_y^{(2)} + \sigma_z^{(1)} \sigma_z^{(2)}$$

This operator always yields a certain information:

$$\langle \Psi_+ | \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} | \Psi_+ \rangle = \text{const}$$

3. Density Matrices

A complete description of the Bell state involves the variables both at Alice and Bob's ends. To evaluate the result of a measurement to be carried out only at, say, Alice's end, we still operate on the whole state, which involves both ends. To capture the complete information

Alice (not Bob) has, we need to introduce new tools: density matrix and reduced density matrix.

We begin our introduction to density matrix with an alternative expression for evaluating the expectation value. First, let us define the **trace (迹)** of an operator L to be

$$\text{Tr} L = \sum_i \langle i | L | i \rangle$$

where $\{|i\rangle\}$ is a complete set of basis vectors.

- The trace of a projection operator is 1.
- The trace of a Hermitian operator is the sum of its eigenvalues.

Recall the completeness condition $\sum_i |i\rangle \langle i| = I$.

$$L = LI = \sum_i L |i\rangle \langle i|$$

The expectation value of L in state $|\psi\rangle$ can be, alternatively, written as

$$\langle \psi | L | \psi \rangle = \sum_i \langle \psi | L | i \rangle \langle i | \psi \rangle = \sum_i \langle i | \psi \rangle \langle \psi | L | i \rangle$$

where we simply reverse the order of the two numbers in the second equality.

According to the definition $\text{Tr} L = \sum_i \langle i | L | i \rangle$,

$$\langle \psi | L | \psi \rangle = \text{Tr} |\psi\rangle \langle \psi| L \equiv \text{Tr} \rho L$$

$\rho \equiv |\psi\rangle \langle \psi|$ is the **density matrix** of the pure state $|\psi\rangle$.

Density matrix can also be used to describe a state of incomplete information.

For example, Charlie has prepared a qubit and sends it to Alice. He does not tell her along which axis the qubit was prepared. Instead, he tells her that the state is equally likely to be $|0\rangle$ along the z axis or $|r\rangle$ along the x axis. Alice can reason that the expectation value of L is

$$\langle L \rangle = \frac{1}{2} \langle 0 | L | 0 \rangle + \frac{1}{2} \langle r | L | r \rangle = \frac{1}{2} \text{Tr} |0\rangle \langle 0| L + \frac{1}{2} \text{Tr} |r\rangle \langle r| L$$

Now we can define a density matrix ρ that encodes Alice's knowledge such that $\langle L \rangle = \text{Tr} \rho L$. One can read that the density matrix ρ is half the projection operator onto $|0\rangle$ plus half the projection operator onto $|r\rangle$

$$\rho = \frac{1}{2} |0\rangle \langle 0| + \frac{1}{2} |r\rangle \langle r|$$

which represents a **mixed state**.

One can generalize $\rho = \sum_i P_i |\psi_i\rangle \langle \psi_i|$ to be a mixture of projection operators with probabilities P_i .

4. Reduced Density Matrix and Entanglement Entropy

4.1 Reduced Density Matrix

Now, for a separable state $|\psi\rangle = |\lambda\rangle_A |\phi\rangle_B$, the density matrix is

$$\rho = |\psi\rangle \langle \psi| = |\lambda\rangle \langle \lambda| \otimes |\phi\rangle \langle \phi| = \rho_A \otimes \rho_B$$

where we can define **reduced density matrices**

$$\rho_A = |\lambda\rangle \langle \lambda|, \quad \rho_B = |\phi\rangle \langle \phi|$$

as the density matrices separately for each subsystem. Notice that $\rho_A^2 = \rho_A$ and, hence, $\text{Tr} \rho_A^2 = 1$.

For an entangled state, it is possible to write (known as the **Schmidt decomposition**)

$$|\psi\rangle = \sum_i c_i |\lambda_i\rangle_A |\phi_i\rangle_B$$

where $\{|\lambda_i\rangle_A\}$ and $\{|\phi_i\rangle_B\}$ orthonormal basis sets for the A and B subsystems, respectively. The reduced density matrices are defined as

$$\begin{aligned} \rho_A &= \text{Tr}_B |\psi\rangle \langle \psi| = \sum_i |c_i|^2 |\lambda_i\rangle \langle \lambda_i| \\ \rho_B &= \text{Tr}_A |\psi\rangle \langle \psi| = \sum_i |c_i|^2 |\phi_i\rangle \langle \phi_i| \end{aligned}$$

In fact, the orthonormal sets $\{|\lambda_i\rangle_A\}$ and $\{|\phi_i\rangle_B\}$ are the eigenstates of the reduced density matrices ρ_A and ρ_B , respectively. Each state $|\lambda_i\rangle$ of the A subsystem is uniquely associated with a state $|\phi_i\rangle$ of the B subsystem with the identical eigenvalue $|c_i|^2$ of the corresponding reduced density matrix. Notice that in the entangled case $\text{Tr} \rho_A^2 = \text{Tr} \rho_B^2 \neq 1$ which can be used to detect bipartite entanglement between A and B subsystems.

4.2 Entanglement Entropy

The von Neumann (Shannon) entropy measures the amount of information. Likewise, we can define **entanglement entropy**

$$S_A = -\text{Tr}_A (\rho_A \log_2 \rho_A) = -\sum_i |c_i|^2 \log_2 |c_i|^2$$

to measure the entanglement of the two subsystems quantitatively. Notice that $S_A = S_B$. Entanglement entropy are widely used these days to understand systems in different phases and through phase transitions.

V Time Evolution of Closed Quantum Systems

1. Time-Evolution Operator

Apply an operator on a state-vector when the system evolves in time. Given the state of a system $|\psi(0)\rangle$ at time $t = 0$, the state of the system at time t can be expressed as

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

where $U(t)$ is called the time-evolution operator. While measurements are probabilistic and irreversible in general, the time evolution of the state-vector is deterministic and reversible.

Principle 5: The evolution of state-vectors with time is unitary, i.e.

$$U^\dagger U = I$$

If U is unitary, and if $|a\rangle$ and $|b\rangle$ are any two state-vectors, then the inner product of $|a'\rangle = U|a\rangle$ and $|b'\rangle = U|b\rangle$ is the same as the inner product of $|a\rangle$ and $|b\rangle$, i.e.

$$\langle a'|b'\rangle = \langle a|U^\dagger U|b\rangle = \langle a|b\rangle$$

- If $|a\rangle$ is normalized, so is $U|a\rangle$.
- If $|a\rangle$ and $|b\rangle$ are distinguishable, i.e. $\langle a|b\rangle = 0$, so are $U|a\rangle$ and $U|b\rangle$. That is, information (or distinction) is never lost.

Consider the time-evolution operator $U(\epsilon)$ for infinitesimal ϵ , and seek a differential equation for the evolution of the state-vector. The operator must satisfy

- Unitarity

$$U^\dagger(\epsilon)U(\epsilon) = I$$

- Continuity

$$U(\epsilon) = U(0) + \frac{\epsilon}{i\hbar} H$$

where $U(0) = I$ and $-\frac{i}{\hbar}$ is included by convention.

Putting them together, we have

$$\left(I + \frac{\epsilon}{i\hbar} H\right)^\dagger \left(I + \frac{\epsilon}{i\hbar} H\right) = I$$

which, in the leading order $O(\epsilon)$, leads to $H^\dagger - H = 0$.

Thus, we find that H defined in the continuity condition is Hermitian, $H^\dagger = H$.

Further, H can be identified as the quantum Hamiltonian. According to the definition,

$$|\psi(t + \epsilon)\rangle = |\psi(t)\rangle + \frac{\epsilon}{i\hbar} H |\psi(t)\rangle$$

Taking the limit as $\epsilon \rightarrow 0$,

$$\lim_{\epsilon \rightarrow 0} \frac{|\psi(t + \epsilon)\rangle - |\psi(t)\rangle}{\frac{\epsilon}{i\hbar}} = i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H |\psi(t)\rangle$$

which is the time-dependent Schroedinger equation.

2. Manipulating Qubits: Rabi Oscillations

2.1 Spin in a Magnetic Field

If we know the Hamiltonian of a system (and its initial state), we can calculate how the state of the system evolves with time. H can be identified with the classical concept of a Hamiltonian, and its eigenvalues with energy. In general, we can derive it from experiment, or borrow it from the classical theory. Sometimes, we can pick one based on symmetry or just experience.

In the case of a single spin, the choice is obvious. All 2×2 Hermitian matrix can be expanded as a linear combination of the identity matrix I and Pauli matrices.

$$\begin{aligned} H &= \begin{pmatrix} a & b \\ c & d \end{pmatrix} = H^\dagger = \begin{pmatrix} \bar{a} & \bar{c} \\ \bar{b} & \bar{d} \end{pmatrix} \\ \therefore H &= \begin{pmatrix} r_1 & \alpha_i \beta \\ \alpha + i\beta & r_2 \end{pmatrix} \\ &= a_1 I + a_2 \sigma_x + a_3 \sigma_y + a_4 \sigma_z \end{aligned}$$

Spin is a 3-vector, and it must find another 3-vector to make a scalar operator H . In the magnetic field, this is the obvious choice, so

$$H \sim -\vec{\sigma} \cdot \vec{B} = -\begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}$$

In particular, we consider a simple example in which $\vec{B} = B_z \hat{z}$. For convenience, we often write

$$H_0 = -\frac{\hbar\omega_0}{2} \sigma_z$$

In which we absorb B_z into the frequency ω_0 .

- The Hamiltonian has two eigenvalues $\pm \frac{\hbar\omega_0}{2}$, and the corresponding eigenstates are $|0\rangle$ and $|1\rangle$.

- The minus sign is a convention, such that $|0\rangle$ or “spin up” is the ground state.
- The system can absorb or emit a photon of energy $\hbar\omega_0$, which can be measured experimentally.

Since H_0 is independent of time, we can solve the time-evolution equation

$$i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = H_0 |\psi(t)\rangle$$

by symbolic integration to give

$$|\psi(t)\rangle \equiv U_0(t) |\psi(0)\rangle = e^{-iH_0 t/\hbar} |\psi(0)\rangle$$

where $|\psi(0)\rangle$ is the state-vector at $t = 0$.

In practice, we find all the eigenvalues and eigenvectors

$$H |j\rangle = E_j |j\rangle$$

Expand the initial state $|\psi_0\rangle$ with the eigenvector basis

$$|\psi(t=0)\rangle = \sum_j |j\rangle \langle j|\psi_0\rangle$$

The evolution of the state-vector is

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

The initial state can be written, in the σ_z basis (in which H_0 is diagonal), as

$$|\psi(0)\rangle = \cos \frac{\theta}{2} |0\rangle + \sin \frac{\theta}{2} |1\rangle$$

The time-evolution operator, in the same basis, is

$$\begin{aligned} U_0(t) &= e^{(-iH_0 t/\hbar)\sigma_z} = e^{i(\omega_0 t/2)\sigma_z} = \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix} \\ &= e^{i\omega_0 t/2} |0\rangle \langle 0| + e^{-i\omega_0 t/2} |1\rangle \langle 1| \end{aligned}$$

Therefore, the state-vector at time t is

$$|\psi(t)\rangle = e^{i\omega_0 t/2} \cos \frac{\theta}{2} |0\rangle + e^{-i\omega_0 t/2} \sin \frac{\theta}{2} |1\rangle$$

Owing to the arbitrary overall phase, we can write

$$|\psi(t)\rangle = \cos \frac{\theta}{2} |0\rangle + e^{-i\omega_0 t} \sin \frac{\theta}{2} |1\rangle$$

The state-vector on the Bloch sphere precesses about \hat{z} -axis with an angular frequency ω_0 .

It is interesting to note that if we absorb the phase into the basis

$$|0\rangle \rightarrow |0'\rangle \equiv e^{i\omega_0 t/2} |0\rangle, \quad |1\rangle \rightarrow |1'\rangle \equiv e^{-i\omega_0 t/2} |1\rangle$$

the state “remains” unchanged as

$$|\psi(t)\rangle = \cos \frac{\theta}{2} |0'\rangle + \sin \frac{\theta}{2} |1'\rangle$$

In other words, in the so-called **rotating reference frame**, the state vector remains unchanged, i.e., the effective Hamiltonian in the rotating frame is $H' = 0$. (将操作旋转到了坐标轴)

2.2 Interaction Picture

In this so-called the interaction picture, the basis is defined, in general, by

$$|n'\rangle = U_0(t) |n\rangle$$

so we redefine the wave function and the observables \hat{O}

$$|\psi_I(t)\rangle = U_0(t)^\dagger |\psi(t)\rangle, \quad \hat{O}_I = U_0(t)^\dagger \hat{O} U_0(t)$$

One can check that the probability density and expectation values remain unchanged

$$\langle n|\psi_I\rangle = \langle n'|\psi\rangle, \quad \langle \psi_I|\hat{O}_I|\psi_I\rangle = \langle \psi|\hat{O}|\psi\rangle$$

In this frame the new wave function is dictated by an interaction-picture Hamiltonian

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} |\psi_I\rangle &= H_I(t) |\psi_I\rangle \\ &= \left[U_0(t)^\dagger H(t) U_0(t) - i\hbar U_0(t)^\dagger \left(\frac{\partial}{\partial t} U_0(t) \right) \right] |\psi_I\rangle \end{aligned}$$

2.3 Manipulating a Spin (Qubit)

A constant $\vec{B} = B_z \hat{z}$ does not transform a state, e.g., from $|0\rangle$ to an arbitrary linear superposition of $|0\rangle$ and $|1\rangle$.

This can be done by applying, in addition to a constant B_z , a magnetic field $\vec{B}_1(t)$ rotating in the x - y plane with angular frequency ω :

$$\vec{B}_1(t) = B_1(\cos \omega t \hat{x} - \sin \omega t \hat{y})$$

such that the Hamiltonian becomes

$$H(t) = -\frac{\hbar\omega_0}{2} \sigma_z - \frac{\hbar\omega_1}{2} (\sigma_x \cos \omega t - \sigma_y \sin \omega t)$$

For microwave controls, we can use the microwave frequency ω in the free rotation $U_0(t) = e^{i(\omega t/2)\sigma_z}$. In the interacting picture, therefore, one can show that

$$\begin{aligned} U_0^\dagger \sigma_z U_0 &= \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{i\omega t/2} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} e^{i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \\ U_0^\dagger \sigma_x U_0 &= \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix} \\ U_0^\dagger \sigma_y U_0 &= \begin{pmatrix} 0 & -ie^{-i\omega t} \\ ie^{i\omega t} & 0 \end{pmatrix} \end{aligned}$$

Therefore, we have, in the rotating frame,

$$\begin{aligned} H_I(t) &= \left[U_0(t)^\dagger H(t) U_0(t) - i\hbar U_0(t)^\dagger \left(\frac{\partial}{\partial t} U_0(t) \right) \right] \\ &= -\frac{\hbar(\omega_0 - \omega)}{2} \sigma_z - \frac{\hbar\omega_1}{2} \sigma_x \end{aligned}$$

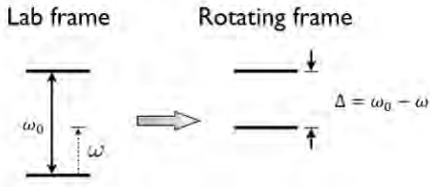


Figure 5: The lab frame and the rotating frame

If at time $t = 0$ the spin is in the state $|0\rangle$, its probability in state $|1\rangle$ at time t can be calculated to be

$$|\langle 1|\psi(t)\rangle|^2 = |\langle 1|\psi_I(t)\rangle|^2 = \left(\frac{\omega_1}{\Omega}\right)^2 \sin^2 \frac{\Omega t}{2}$$

where $\Omega = \sqrt{(\omega - \omega_0)^2 + \omega_1^2}$.

This is the phenomenon of **Rabi oscillations**, which is the basic process to manipulate qubits in quantum computing. These oscillations are obtained by exposing qubits to periodic electromagnetic fields during suitably adjusted time intervals.

3. Recap of the Quantum Theory in General Physics

The state of a quantum particle is represented by a wave function $\psi(\vec{r}, t)$.

The time evolution of the state $\psi(\vec{r}, t)$ of a non-relativistic particle is governed by the Schroedinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

where the Hamiltonian for conserved forces is

$$H = -\frac{\hbar^2}{2m} \nabla^2 + U(\vec{r}, t)$$

where H is independent of time, the wave function can be separated to be $\psi(\vec{r}, t) = \phi(\vec{r})e^{-iEt/\hbar}$, which satisfies

$$H\phi = E\phi$$

The probability of finding the particle somewhere at a particular time is proportional to $|\psi(\vec{r}, t)|^2$. A particle in a potential trap is only allowed to have discrete energy levels. The particle can absorb light and gain energy or emit light and lose energy. Only photons whose energies (or colors) match the “jump” in energy levels can be emitted or absorbed.

We have encountered the following wave functions to describe the state of a particle.

- A 1D particle localized at $x = x_0$ has a wave function $\psi(x) = \delta(x - x_0)$, where $\delta(x)$ is the Dirac delta function. This is a real-space eigenstate.
- A particle moving along the x direction with momentum $\hbar k$ has a wave function $\psi(x) = e^{ikx}$. This is a momentum-space eigenstate.
- The electron in the ground state of a hydrogen atom has a wave function $\psi(\vec{r}) = e^{-r/a_B}$, where a_B is the Bohr radius. This is neither a real-space eigenstate nor a momentum-space eigenstate.

3.1 Heisenberg vs Schroedinger

- 1) Heisenberg invented one with vectors, linear operators and their algebra.
- 2) Schroedinger thought in terms of wave functions and wave equations.

The two approaches can be united: wave functions form a vector space, while derivatives are operators.

3.2 What are Wave Functions, Really?

Suppose we have an orthogonal basis labelled by $|a, b, c, \dots\rangle$, where a, b, c, \dots are eigenvalues of some complete set of commuting observables A, B, C . An arbitrary

state vector can be expanded as

$$|\Psi\rangle = \sum_{a,b,c,\dots} \psi(a,b,c,\dots) |a,b,c,\dots\rangle$$

The set of coefficients $\psi(a,b,c,\dots) = \langle a,b,c,\dots|\Psi\rangle$ is called the **wave function** of the system in the basis defined by the observables A, B, C, \dots .

We can only choose labels that are not conflicting. In the quantum theory, this means observables A and B commute, i.e., $[A, B] \equiv AB - BA = 0$. As a consequence,

$$AB|a,b,c,\dots\rangle = BA|a,b,c,\dots\rangle = ab|a,b,c,\dots\rangle$$

The probability for the commuting observables to have values a, b, c, \dots is

$$P(a,b,c,\dots) = \psi^*(a,b,c,\dots)\psi(a,b,c,\dots)$$

with

$$\sum_{a,b,c,\dots} \psi^*(a,b,c,\dots)\psi(a,b,c,\dots) = 1$$

4. Continuous Functions as Vectors

It can be shown that complex functions form a complex vector space, or a **Hilbert space**.

But to translate the principles of quantum mechanics between vector-based ideas (Heisenberg) to function-oriented ideas (Schrodinger), we need the following recognitions

- 1) Integral replace sum.
- 2) Dirac delta function replace Kronecker delta.
- 3) Probability density replace probability.

4.1 Integral Replace Sum

Consider a ket-vector $|\psi\rangle = \sum_i \alpha_i |i\rangle$. The basis $|i\rangle$ gets translated to a continuous basis $|x_i\rangle$, which describes a particle at x_i . The analogy to the state vector is (notice $\sum_i \rightarrow \int dx$)

$$|\psi\rangle = \int dx_i \psi(x_i) |x_i\rangle$$

Therefore, the wave function, as the coefficient $\alpha_i = \langle i|\psi\rangle$, is

$$\psi(x) = \langle x|\psi\rangle$$

Strictly speaking, $\psi(x)$ isn't a state, which we call $|\psi\rangle$.

4.2 Dirac Delta Function Replace Kronecker Delta

To have the algebra self-consistent, we have

$$\psi(x) = \langle x|\psi\rangle = \int dx_i \psi(x_i) \langle x|x_i\rangle$$

In the vector-based description, $\langle j|i\rangle = \delta_{ij}$. It is natural to identify $\langle x|x_i\rangle = \delta(x - x_i)$, the Dirac delta function, which satisfies

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

$$\int_{-\infty}^{\infty} f(x') \delta(x - x') dx' = f(x)$$

Thus, we can interpret $\langle x_i|x_j\rangle = \delta(x_i - x_j)$ as the orthogonality of the basis vectors.

4.3 Probability Density Replace Probability

The normalization of the ket-state is

$$\langle \psi|\psi\rangle = \sum_i \langle \psi|i\rangle \langle i|\psi\rangle = \sum_i \alpha_i^\dagger \alpha_i = 1$$

where we have inserted the completeness condition $\sum_i |i\rangle \langle i| = 1$.

The continuum version would be

$$\langle \psi|\psi\rangle = \int dx \langle \psi|x\rangle \langle x|\psi\rangle = \int dx \psi^*(x) \psi(x) = 1$$

We can identify the completeness condition as, symbolically

$$\int dx |x\rangle \langle x| = 1$$

The product $\psi^*(x)\psi(x)$ is known as the **probability density**.

VI From the Microscopic to the Macroscopic World

1. (No-)Cloning of the Quantum States

Getting from One to Two (and More). What extent can we duplicate the information of a quantum state.

1) The first possibility is to copy or clone, as if we had a quantum copy machine. Putting in a qubit in a state $|\psi\rangle = \mu|0\rangle + \nu|1\rangle$, we would get a new qubit in the state $|\psi\rangle = \mu|0\rangle + \nu|1\rangle$ and the original qubit in the state $|\psi\rangle$ back. In other words, the result is

$$|\psi\rangle|\psi\rangle = \mu^2|0\rangle|0\rangle + \mu\nu|0\rangle|1\rangle + \nu\mu|1\rangle|0\rangle + \nu^2|1\rangle|1\rangle$$

2) The second possibility is to entangle, which we have learned in Lecture 4. Given a quantum state $|\psi\rangle = \mu|0\rangle + \nu|1\rangle$ and another qubit, say, in the state $|0\rangle$, we obtain $\mu|0\rangle|0\rangle + \nu|1\rangle|1\rangle$.

Theorem VI.1 (The No-Cloning Theorem)

It is not possible to perfectly clone an unknown quantum state, or a state drawn from a set of two (or more) non-orthogonal states.

2. The Process of Measurement

Unlike in classical computation, entanglement is a fundamentally new resource crucial in quantum error correction and quantum parallelism.

Quantum measurement generally encounter entanglement between microscopic and macroscopic systems, such as an atom (with spin) and a Stern-Gerlach apparatus.

In the simplest description, the apparatus has exactly three states: a blank state $|b\rangle$ and two outcome states $|u\rangle$, $|d\rangle$. Coupled with the spin state $|0\rangle$, $|1\rangle$, the combined system has six basis vectors. Measurement involves interaction between (hence, joint evolution of) spin and the apparatus, so we have, e.g.,

$$\begin{aligned} |0b\rangle &\rightarrow |0u\rangle \\ |0b\rangle &\rightarrow |1d\rangle \\ \alpha_0|0b\rangle + \alpha_1|1b\rangle &\rightarrow \alpha_0|0u\rangle + \alpha_1|1d\rangle \end{aligned}$$

In general, the entanglement between the spin and the apparatus occurs via a unitary evolution of the state-vector. There is no wave function collapse at this stage.

3. The Schroedinger Cat Paradox

Schroedinger (1935) dramatize it by introducing a fictitious cat, whose living and dead states are entangled to the atomic states in a radiative decay:

$$|\psi_{A+C}\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle|0_C\rangle + |1_A\rangle|1_C\rangle)$$

It turns out when we come to the macroscopic world, the cat state is really coupled to a large environment E (the whole cat and its surrounding). The whole system (if we assume the environment is initially in a pure state) is, e.g.,

$$|\psi_{A+C+E}\rangle = \frac{1}{\sqrt{2}}(|0_A\rangle|0_C\rangle|\zeta_E^0\rangle + |1_A\rangle|1_C\rangle|\zeta_E^1\rangle)$$

The coupling to the environment functions as a measurement, which leaks the information of the living or dead state, even though human observers are not looking. In other words, the presence of a large object (the real cat) at different macroscopic states (e.g., positions of the cat) influences the microscopic state, so the coherence between the living and dead states associated to, e.g., different positions vanishes (hence the name decoherence). As a result, the environmental measurement prevents interference effects from building up between the living and dead states. Very quickly, the cat is either dead or alive and not in a superposition of the two states. (不存在叠加态, 叠加态因为环境作用退相干为经典了)

4. Quantum LC Oscillator

4.1 Quantum Electrical Circuits

Once we summarize the device properties by a set of operating parameters (which are determined by quantum physics), we can operate it classically, because the collective degrees of freedom (such as current I and voltage V) are pure classical—they are numbers, not quantum operators.

On the other hand, intrinsically quantum mechanical circuit elements can be achieved in superconducting electrical circuits. They have quantized energy levels and can be set up into the quantum superpositions of different energy states. We discuss the theory of quantum LC oscillators here, but leave superconductivity to later lectures.

4.2 The Harmonic Oscillator

In classical physics, a block attached to a spring, a pendulum, or the electric current in an LC circuit can be described as a harmonic oscillator.

All these systems, when disturbed, oscillate about the equilibrium point—any smooth energy function looks like a parabola close to its minimum. The energy of a block of mass m attached to a spring with strength k is

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

The classical equation of motion for a harmonic oscillator is given by

$$\frac{d^2x}{dt^2} + \omega^2x = 0$$

where the characteristic frequency of oscillation is $\omega = \sqrt{\frac{k}{m}}$.

The general solution is

$$x(t) = A \cos \omega t + B \sin \omega t$$

When we differentiate it twice, we obtain a factor of $-\omega^2$.

4.3 Quantum LC Oscillator

The total energy of an LC circuit is,

$$E = \frac{1}{2}L\dot{q}^2 + \frac{q^2}{2C} = \frac{1}{2}L\dot{q}^2 + \frac{q^2}{2C}$$

We can treat q as the position coordinate of a block with ‘mass’ L and ‘spring constant’ $1/C$.

In this analogy the momentum coupled to the charge is

$$L\dot{q} = LI = \Phi$$

which is the flux through the inductor.

For the convenience of later discussion with Josephson junctions, which act as nonlinear inductors, we take the node flux to be the coordinate. The node flux is defined by

$$\phi(t) = \int^t d\tau V(\tau)$$

such that the potential difference across the capacitor is $V(t) = \dot{\phi}$.

The total energy becomes, in this new representation,

$$E = \frac{1}{2}C\dot{\phi}^2 + \frac{\phi^2}{2L}$$

This is an oscillator with ϕ as the position coordinate of the block with ‘mass’ C and ‘spring constant’ $1/L$. The momentum coupled to the node flux ϕ reads

$$C\dot{\phi} = CV = Q$$

which is the charge with the sign convention chosen above.

The conditions that an LC oscillator circuit fabricated with the technology of microelectronic chip can be treated as a macroscopic quantum system is

Lumped element assumption (one collective degree of freedom):

- 1) The typical parameters are $L = 10\text{nH}$ and $C = 1\text{pF}$.
- 2) They lead to a resonant frequency $\omega_0/(2\pi) \simeq 1.6\text{GHz}$ in the microwave range.
- 3) The size of the circuit is a few hundred nm, much less than the microwave wavelength.

Negligible environmental effects:

- 1) Dilution fridge: $T \approx 20\text{mK}$, so $k_B T \ll \hbar\omega_0$.
- 2) Superconducting circuit, low dissipation.
- 3) High quality factor reduces the influence of the measuring environment (modeled by an admittance $Y(\omega)$ in parallel) of the LC oscillator.

5. Operator Algebra of Harmonic Oscillators

For quantum harmonic oscillators, we need to solve the time-independent 1D Schrodinger equation

$$H\psi(x) = \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{m\omega^2}{2} x^2 \right] \psi(x) = E\psi(x)$$

with a parabolic potential $U(x) = \frac{m\omega^2}{2} x^2$.

To solve the equation, we must find the allowed functions that satisfy both the differential equation and the boundary conditions $[\psi(\pm\infty) = 0]$, and the corresponding energies E .

In the following, we introduce a pair of ladder operators a, a^\dagger to solve the eigenstate problem.

- 1) The energy levels are equally spaced, like a ladder,

$$E_n = \left(n + \frac{1}{2} \right) \hbar\omega$$

2) The corresponding wave functions are Gaussian tapered:

$$\psi_n(x) = e^{-\frac{m\omega}{2\hbar}x^2} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right)$$

where $H_n(x)$ is a Hermite polynomial.

5.1 Algebraic Solution with Ladder Operators

Begin with the Hamiltonian

$$H = \frac{P^2 + m^2\omega^2 X^2}{2m}$$

Rewrite this as [notice $a^2 + b^2 = (a + ib)(a - ib)$]

$$H \approx \frac{1}{2m} (P + im\omega X)(P - im\omega X)$$

But

$$(P + im\omega X)(P - im\omega X) = (P^2 + m^2\omega^2 X^2) + i\omega(XP - PX)$$

Recall X and $P = i\hbar \frac{d}{dx}$ are operators (matrices). They do not commute. In fact,

$$[X, P] \equiv XP - PX = i\hbar$$

So we have

$$H = \frac{1}{2m} (P + im\omega X)(P - im\omega X) + \frac{1}{2}\hbar\omega$$

This motivates us to define two new operators

$$a = \frac{i}{\sqrt{2m\omega\hbar}} (P - im\omega X)$$

$$a^\dagger = \frac{-i}{\sqrt{2m\omega\hbar}} (P + im\omega X)$$

They are called the lowering and raising operators, which are Hermitian conjugates of each other. We can also define a Hermitian operator $N = a^\dagger a$. They satisfy the following commutation relations

$$[a, a^\dagger] \equiv aa^\dagger - a^\dagger a = 1$$

$$[a, N] = aN - Na = a$$

$$[a^\dagger, N] = a^\dagger N - Na^\dagger = -a^\dagger$$

With these operators, we can write

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

We will first show that the ground-state energy is $E_0 = \frac{\hbar\omega}{2}$

Assume we know the ground state $|\psi_0\rangle$, and

$$N |\psi_0\rangle = N_0 |\psi_0\rangle$$

1) From $[a, N] = a$, we have $Na = a(N - 1)$. So,

$$N(a |\psi_0\rangle) = a(N - 1) |\psi_0\rangle = (N_0 - 1)(a |\psi_0\rangle)$$

2) This appears to imply that $a |\psi_0\rangle$ is an eigenstate of N with eigenvalue $N_0 - 1$; this cannot be true, as we assumed the eigenvalue of the ground state to be N_0 . To avoid contradiction, we must have $a |\psi_0\rangle = 0$, i.e., $|\psi_0\rangle$ is annihilated by a .

3) Therefore, we must have $N_0 = 0$, as

$$N |\psi_0\rangle = a^\dagger a |\psi_0\rangle = 0$$

Up to a constant factor, this yields, for the ground state wave function $\psi_0(x)$

$$(P - im\omega X)\psi_0(x) = 0$$

Replacing P by $-i\hbar \frac{d}{dx}$, we obtain

$$\frac{d\psi_0}{dx} = -\frac{m\omega X}{\hbar} \psi_0(x)$$

The differential equation can be satisfied, indeed, by

$$\psi_0(x) = e^{-\frac{m\omega}{2\hbar}x^2}$$

Now, knowing the ground state $|\psi_0\rangle$, we can write down all eigenstates (labeled by $|\psi_n\rangle$) through iteration.

1) From $[a^\dagger, N] = -a^\dagger$, we have

$$Na^\dagger = a^\dagger(N + 1)$$

or $N(a^\dagger |\psi_n\rangle) = a^\dagger(N + 1) |\psi_n\rangle$

2) For $n = 0$, we define $|\tilde{\psi}_1\rangle = a^\dagger |0\rangle$ and find

$$N |\tilde{\psi}_1\rangle = N(a^\dagger |\psi_0\rangle) = a^\dagger(N + 1) |\psi_0\rangle = a^\dagger |\psi_0\rangle = |\tilde{\psi}_1\rangle$$

In other words, the eigenvalue of N is 1 for $|\tilde{\psi}_1\rangle$.

3) We can continue to iterate and obtain, in general, $|\tilde{\psi}_n\rangle = a^\dagger |\tilde{\psi}_{n-1}\rangle$ with n being the eigenvalue of N .

The eigenstates $|\tilde{\psi}_n\rangle$ are not normalized. In fact,

$$\langle \tilde{\psi}_1 | \tilde{\psi}_1 \rangle = \langle \psi_0 | aa^\dagger | \psi_0 \rangle = \langle \psi_0 | a^\dagger a + 1 | \psi_0 \rangle = 1$$

$$\langle \tilde{\psi}_2 | \tilde{\psi}_2 \rangle = \langle \psi_1 | aa^\dagger | \psi_1 \rangle = \langle \psi_1 | a^\dagger a + 1 | \psi_1 \rangle = 2$$

$$\vdots$$

$$\langle \tilde{\psi}_n | \tilde{\psi}_n \rangle = \langle \psi_{n-1} | aa^\dagger | \psi_{n-1} \rangle = \langle \psi_{n-1} | a^\dagger a + 1 | \psi_{n-1} \rangle = n!$$

where we used $[a, a^\dagger]aa^\dagger - a^\dagger a = 1$.

Therefore, we can define normalized eigenstates as

$$|n\rangle \equiv |\psi_n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}} |\psi_0\rangle$$

Therefore, we just solve the eigenvalue problem of $H = \hbar\omega(N + \frac{1}{2})$. The eigenenergies are (called a ladder)

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots$$

The eigenstates satisfy

$$\begin{aligned} a^\dagger |n\rangle &= \sqrt{n+1} |n+1\rangle \\ a |n\rangle &= \sqrt{n} |n-1\rangle \\ N |n\rangle &= a^\dagger a |n\rangle = a^\dagger \sqrt{n} |n-1\rangle = n |n\rangle \end{aligned}$$

Therefore, the operator method can replace solving the Schroedinger equation completely. All wave functions can be obtained by the operator algebra.

1) Up to a constant factor, we have

$$\psi_1(x) \sim (P + im\omega X)\psi_0(x) \sim \left(\sqrt{\frac{m\omega}{\hbar}} x \right) \psi_0(x)$$

2) Similarly, we have

$$\begin{aligned} \psi_2(x) &\sim (P + im\omega X)\psi_1(x) \\ &\sim \left[2 \left(\sqrt{\frac{m\omega}{\hbar}} x \right)^2 - 1 \right] \psi_0(x) \end{aligned}$$

The polynomials of $\sqrt{m\omega/\hbar}x$ are known as **Hermite polynomials** $H_n(x)$.

VII From Digital Electronics to Quantum Computers

1. Digital Electronics

$A, B, \bar{A}, A \cdot B, A + B$.

ALU. 但量子不可克隆, 所以任何分支都不太行.

2. Quantum Gates

A quantum gate is a reversible operation that a quantum computer can perform upon qubits.

A gate is a linear transformation on the state of the qubit that takes unit vectors into unit vectors. Such a transformations u is called **unitary** and satisfies the condition

$$uu^\dagger = u^\dagger u = 1$$

We begin with single-qubit gates. Note that the NOT operation X is the only nontrivial reversible operation a classical computer can perform on a single bit.

1) NOT gate (Pauli X matrix):

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$X |0\rangle = |1\rangle$$

$$X |1\rangle = |0\rangle$$

NOT gate flips the qubit, just like a classical bit.

2) Hadamard gate can flip the qubit half way, such that we have a superposition of 0 and 1.

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \sim \sqrt{NOT}$$

$$H |0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$H |1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

Hadamard gates are often used to implement quantum parallelism.

3) We can also shift the phase of the qubit by a rotation around z axis. Pauli Z matrix:

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

$$Z(a |0\rangle + b |1\rangle) = a |0\rangle - b |1\rangle$$

Next, we discuss the quantum version of a controlled-NOT (CNOT) gate, which is a two-qubit gate. (可以提供纠缠)

- If the state of the i th qubit (the control qubit) is $|0\rangle$, C_{ij} leaves the state of the j th qubit (the target qubit) unchanged.
 - If the state of the control qubit is $|1\rangle$, C_{ij} applies the NOT operator X to the state of the target qubit.
- e.g.

$$C_{12}(a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle) \\ = a|00\rangle + b|01\rangle + c|11\rangle + d|10\rangle$$

Matrix representation:

$$C_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad C_{21} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

3. Application: Quantum Teleportation

Teleportation is not the transfer of an object by disappearing it from one point in space and reappearing it in another location. It is a transfer of the information that fully characterizes all properties of the object.

Suppose Alice has a qubit in an unknown state $|\psi\rangle_A = a|0\rangle + b|1\rangle$. In teleportation, her goal is to transfer the information (i.e. a and b), not the physical qubit, to Bob at a different location.

(这里的分支相当于不变的演化)

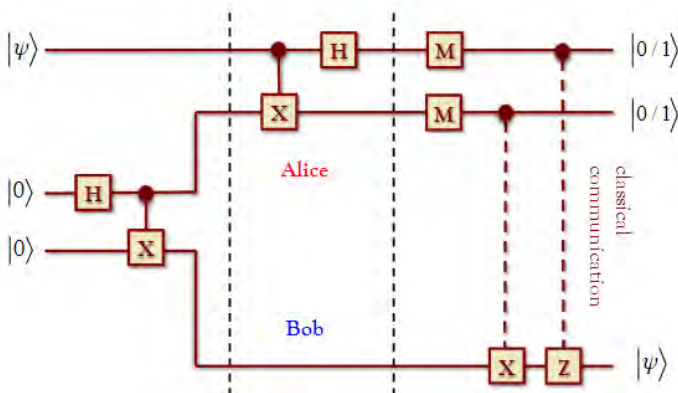


Figure 6: Quantum Teleportation

After Stage 1:

$$|\Psi\rangle = (a|0\rangle + b|1\rangle) \otimes \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \\ = \frac{1}{\sqrt{2}}(a|000\rangle + a|011\rangle + b|100\rangle + b|111\rangle)$$

After Stage 2:

$$|\Psi\rangle = \frac{1}{2}(a|000\rangle + a|100\rangle + a|011\rangle + a|111\rangle + \\ b|010\rangle - b|110\rangle + b|001\rangle - b|101\rangle) \\ |\Psi\rangle = \frac{1}{2}[|00\rangle(a|0\rangle + b|1\rangle) + |01\rangle(a|1\rangle + b|0\rangle) + \\ |10\rangle(a|0\rangle - b|1\rangle) + |11\rangle(a|1\rangle - b|0\rangle)]$$

$$|\Psi\rangle = \frac{1}{2}[|00\rangle I + |01\rangle X + |10\rangle Z + |11\rangle XZ](a|0\rangle + b|1\rangle)$$

Alice has no knowledge of the quantum state, even though she is able to teleport it.

Nor does Alice maintain a copy of the quantum state. After the teleportation, the original qubit ends up either in $|0\rangle$ or $|1\rangle$, depending on the measurement result.

The classical communication channel is limited by the speed of light, so quantum teleportation cannot be accomplished faster than the speed of light.

4. Toward a Working Quantum Computer

- Josephson junctions
- Trapped ions
- Photons
- Quantum dots
- NMR
- NV-centers in diamond
- Rydberg atom arrays
- Impurity spins in semiconductors
- Atoms and cavity QED
- Majoranas in quantum wires
- and more . . .

Five criteria for physical implementation of a quantum computer:

- 1) Well defined extendible qubit array-stable memory
- 2) Preparable in the “000...” state
- 3) Long decoherence time ($> 10^4$ operation time)
- 4) Universal set of gate operations
- 5) Single-quantum measurements

4.1 Universal Quantum Gates

A set of gates is said to be universal for quantum computation if any unitary operation may be approximated to arbitrary accuracy by a quantum circuit involving only those gate.

- 1) Any single-qubit unitary transformation can be approximated.
- 2) Any two-qubit unitary transformation can be approximated.
- 3) Any multi-qubit unitary transformation can be decomposed into a circuit of single- and two-qubit gate

An example of a standard set is:

$$\begin{aligned} \text{Hadamard gate: } H &= \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ \frac{\pi}{4} \text{ (phase) gate: } S &= \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} \text{ (not necessary)} \\ &= e^{i\pi/4} \begin{pmatrix} e^{-i\pi/4} & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \\ \frac{\pi}{8} \text{ gate: } S &= \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix} \\ &= e^{i\pi/8} \begin{pmatrix} e^{-i\pi/8} & 0 \\ 0 & e^{i\pi/8} \end{pmatrix} \\ \text{CNOT gate: } C_{12} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \end{aligned}$$

4.2 Superconducting Circuits

A Cooper pair box qubit has a voltage source biasing the box through a coupling ('gate') capacitor. Tunable by gate and flux.

Circuit QED engineers superconducting qubits as artificial atoms coupled to microwave resonators (typically, with a single mode).

4.3 Fault-Tolerant Quantum Computing

Redundancy in coding offers possibilities to detect errors.

Microsoft is supporting a completely new quantum computing scheme, in which information is store globally in the wave function topology of an engineered system.

4.4 Quantum Algorithm

Early algorithms provided clear, but often not practical, evidences that quantum advantages exist. Quantum supremacy using a programmable superconducting processo.

In the so-called NISQ era, hybrid classical-quantum algorithms may greatly enhance our computational capabilities (perhaps, with a probability).

VIII Quantum Algorithms

1. Reversibility and Quantum Parallelism

1.1 The General Computational Process

A computation is a map

$$f : x \leftarrow f(x)$$

where x is an n -bit integer, and $f(x)$ is an m -bit integer. The total resources are at least, $n + m$ qubits.

In a quantum computer, the computation is achieved by applying a unitary transformation U_f to the $n + m$ qubits.

$$U_f(|x\rangle_n |y\rangle_m) = |x\rangle_n |y \oplus f(x)\rangle_m$$

where \oplus represents the bitwise exclusive OR, or mod-2 addition. For example,

$$110010 \oplus 010101 = 100111$$

1.2 Reversibility

The computation is reversible

$$\begin{aligned} U_f U_f(|x\rangle_n |y\rangle_m) &= U_f(|x\rangle_n |y \oplus f(x)\rangle_m) \\ &= |x\rangle_n |y \oplus \underbrace{f(x) \oplus f(x)}_{\forall z, z \oplus z = 0}\rangle_m \\ &= |x\rangle_n |y\rangle_m \end{aligned}$$

In particular, when $y = 0$,

$$U_f(|x\rangle_n |0\rangle_m) = |x\rangle_n |f(x)\rangle_m$$

1.3 Quantum Parallelism

Let us illustrate why, in principle, a quantum computer can achieve superior performance to their classical counterpart.

$$\begin{aligned} H|0\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ H \otimes H(|0\rangle \otimes |0\rangle) &= (H|0\rangle) \otimes (H|0\rangle) \\ &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ &= \frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle) \end{aligned}$$

In general,

$$H^{\otimes n}|0\rangle_n = \frac{1}{2^{n/2}} \sum_{0 \leq x < 2^n} |x\rangle_n$$

where $H^{\otimes n} = \underbrace{H \otimes H \otimes \cdots \otimes H}_{n \text{ times}}$.

Therefore, we seem to calculate in parallel universes.

$$\begin{aligned} U_f(H^{\otimes n} \otimes I_m)(|0\rangle_n |0\rangle_m) &= \frac{1}{2^{n/2}} \sum_{0 \leq x < 2^n} U_f(|x\rangle_n |0\rangle_m) \\ &= \frac{1}{2^{n/2}} \sum_{0 \leq x < 2^n} |x\rangle_n |f(x)\rangle_m \end{aligned}$$

The quantum advantage is that the (unknown) state encodes the possibilities of extracting the information of $f(x)$ for all x . But how do we find out what the state is?

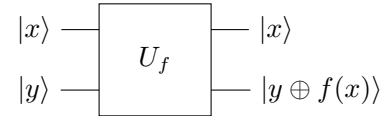
Fortunately, it is sufficient to show that a quantum computer can perform tricks, though in very limited cases, that no classical computer can accomplish. As examples, we will cover

- 1) Deutsch's algorithm
- 2) Grover's search algorithm

2. Deutsch's Trick

2.1 The Deutsch Problem

There exist only four different 1-qubit functions:



The four functions are 0, x , \bar{x} , 1. Or explicitly, notice that, with the truth table or the Venn diagram, one can prove

$$A \oplus B = \overline{A} \oplus \overline{B}$$

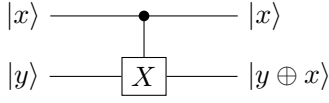
- 1) $U_f = I_4$:

$$f_1(0) = f_1(1) = 0$$

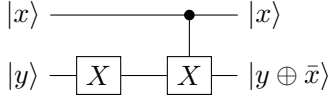
$$\begin{aligned} |x\rangle &\text{—————} |x\rangle \\ |y\rangle &\text{—————} |y \oplus 0\rangle \end{aligned}$$

- 2) $U_f = CNOT$:

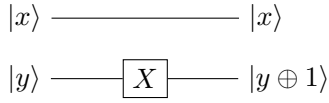
$$f_2(0) = 0, f_2(1) = 1$$



- 3) $U_f = CNOT(I_2 \otimes X)$:
 $f_3(0) = 1, f_3(1) = 0$



- 4) $U_f = (I_2 \otimes X)$:
 $f_4(0) = f_1(1) = 1$

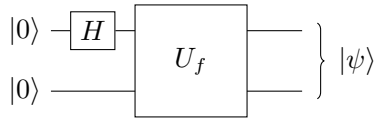


Suppose that we are given a blackbox that executes U_f for one of the four functions. What can we learn about f , if we let the box act once?

Remarkably, with a quantum computer we do not have to run U_f twice to determine whether or not f is a constant.

2.2 An Intuitive Trial

The standard trick, as we discussed on quantum parallelism, is to put the input qubit into the equal superposition of $|0\rangle$ and $|1\rangle$ before the application of U_f .



We obtain

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle |f(0)\rangle + |1\rangle |f(1)\rangle)$$

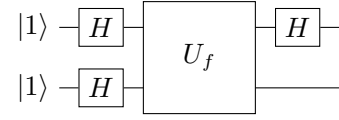
By applying Hadamards to both qubits we obtain

$$\begin{aligned} f_1(0) = f_1(1) = 0, H \otimes H |\psi\rangle &= \frac{1}{\sqrt{2}} |0\rangle (|0\rangle + |1\rangle) \\ f_2(0) = 0, f_2(1) = 1, H \otimes H |\psi\rangle &= \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \\ f_3(0) = 1, f_3(1) = 0, H \otimes H |\psi\rangle &= \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) \\ f_4(0) = f_4(1) = 1, H \otimes H |\psi\rangle &= \frac{1}{\sqrt{2}} |0\rangle (|0\rangle - |1\rangle) \end{aligned}$$

Now measure both qubits. Half the time we obtain 00 and know nothing. Half the time, we either get 01, so $f(0) = f(1)$, or 11, so $f(0) \neq f(1)$. We have a 50% chance of success; one cannot do any better by replacing $H \otimes H$ by other operators.

2.3 The Deutsch Algorithm

A 100%-effective method is the following.



The result is

$$\begin{aligned} U_f(H|1\rangle \otimes H|1\rangle) &= U_f \left[\frac{1}{2} (|00\rangle - |01\rangle - |10\rangle + |11\rangle) \right] \\ &= \frac{1}{2} [|0f(0)\rangle - |1f(1)\rangle \\ &\quad - |0(1 \oplus f(0))\rangle + |1(1 \oplus f(1))\rangle] \\ &= \frac{1}{2} [|0\rangle (|f(0)\rangle - |1 \oplus f(0)\rangle) \\ &\quad + |1\rangle (-|f(1)\rangle + |1 \oplus f(1)\rangle)] \end{aligned}$$

Apply Hadamards to first qubit,

$$\begin{aligned} |\psi\rangle &= \frac{1}{2\sqrt{2}} [(|0\rangle + |1\rangle)(|f(0)\rangle - |1 \oplus f(0)\rangle) \\ &\quad + (|0\rangle - |1\rangle)(-|f(1)\rangle + |1 \oplus f(1)\rangle)] \\ &= \begin{cases} |1\rangle \frac{1}{\sqrt{2}} [|f(0)\rangle - |1 \oplus f(0)\rangle] & f(0) = f(1) \\ |0\rangle \frac{1}{\sqrt{2}} [|f(0)\rangle - |1 \oplus f(0)\rangle] & f(0) \neq f(1) \end{cases} \end{aligned}$$

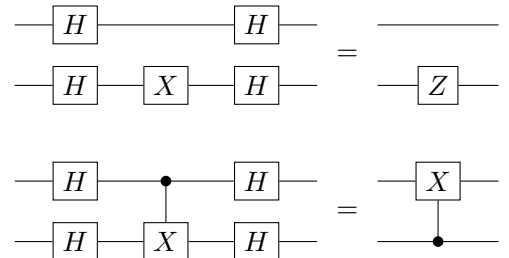
which can be distinguished by measuring the input qubit.

The final state of the output qubit is

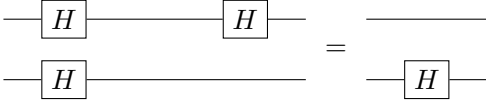
$$\begin{cases} \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle) & f(0) = 0 \\ \frac{1}{\sqrt{2}} (|1\rangle - |0\rangle) & f(0) = 1 \end{cases}$$

Therefore, we don't have any information on $f(0)$, because we always measure $|0\rangle$ or $|1\rangle$ with equal probabilities. The sign difference is not detectable.

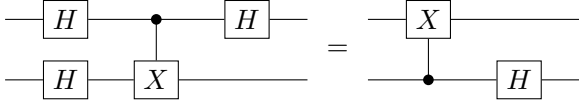
Recall there are equivalent circuits in quantum circuits



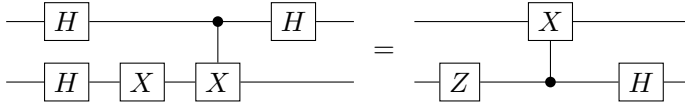
1) $f(x) = 0$



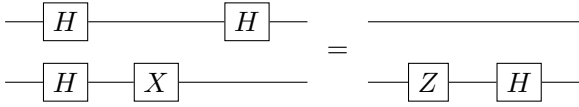
2) $f(x) = x$



3) $f(x) = \bar{x}$



4) $f(x) = 1$



3. Grover's Trick

3.1 The Grover Search Algorithm

The Grover search algorithm performs a search for an entry in an unstructured database, e.g., the title of a book in a library ordered by first author's name.

The normal setup of the problem assumes that we have been given a subroutine that returns

$$f(x) = 0, \quad x \neq a$$

$$f(x) = 1, \quad x = a$$

for any n -bit integer x , where a is the special value being sought.

In practice, it is told that we are given a black box, which is often called an oracle, containing a quantum circuit (which we do not know in general) that implement the function. The oracle incorporates the usual quantum-computational trick that applies a unitary transformation U_f on an n -qubit input and a 1-qubit output as

$$U_f(|x\rangle_n |y\rangle_1) = |x\rangle_n |y \oplus f(x)\rangle_1$$

such that the output isn't flipped or is flipped from 0 to 1 (or vice versa), depending on whether $x = a$ or not.

We are supposed to start from some quantum state. By repeatedly calling the oracle, we manage to evolve the state toward the unknown $|a\rangle$ —so we find it.

If the number of entries in the database is N , which can be encoded by n qubits (i.e., $N \lesssim 2^n$).

The Grover algorithm, as we will show, can solve the problem in $\sim \sqrt{N}$ operations. This is an appreciable, though not exponential, speed-up.

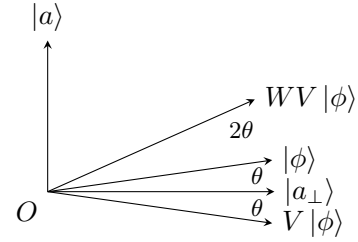
3.2 Geometrical Picture

We use vectors in a two-dimensional plane to illustrate the algorithm. Suppose $|a\rangle$ is the state we want to search. Define $|a_\perp\rangle$ to be the state orthogonal to $|a\rangle$.

Let us introduce an auxiliary state

$$|\phi\rangle = \cos \theta |a_\perp\rangle + \sin \theta |a\rangle$$

where θ is the angle between $|\phi\rangle$ and $|a_\perp\rangle$.



We introduce a reflection V with respect to the direction of $|a_\perp\rangle$ as

$$V = 2 |a_\perp\rangle \langle a_\perp| - I = I - 2 |a\rangle \langle a|$$

The operation flips the sign of the $|a\rangle$ component, while leaving unchanged the components perpendicular to $|a\rangle$.

We can also introduce a reflection W with respect to the direction of $|\phi\rangle$ as

$$W = 2 |\phi\rangle \langle \phi| - I$$

The product of the two reflections is a rotation: WV rotates a vector through the angle 2θ in the direction from $|a_\perp\rangle$ to $|\phi\rangle$.

Each subsequent application of WV increases the angle between the final state and $|a_\perp\rangle$ by another 2θ . A proper choice of the number of WV applications can approach $|a\rangle$ with an error in angle no more than θ .

3.2.1 How to Relate V to the Oracle? How does the oracle fit into the algorithm that repeatedly rotates a quantum state? The answer is that the reflection of V can be straightforwardly implemented with a call of the black box U_f .

$$V|x\rangle = \begin{cases} |x\rangle & x \neq a \\ -|a\rangle & x = a \end{cases}$$

This is nothing but $(-1)^{f(x)}|x\rangle$, so we need a trick to make the effect of U_f merely a sign change.

This is done by initializing the output qubit into the state

$$H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

before the application of U_f .

Convince myself that

$$U_f(|x\rangle \otimes H|1\rangle) = (-1)^{f(x)}|x\rangle \otimes H|1\rangle$$

Interestingly, the application of U_f on the output qubit can be regarded as the identity, so it is never entangled with the input qubits and remains a constant state throughout the algorithm.

Therefore, for an arbitrary n -qubit input state $|\Psi\rangle = \sum_x \alpha_x |x\rangle$, we have explained how to implement

$$U_f(|\Psi\rangle \otimes H|1\rangle) = [|\Psi\rangle - 2|a\rangle\langle a|\Psi\rangle] \otimes H|1\rangle$$

3.2.2 How to Choose $|\phi\rangle$ and Construct W ? Now, the construction of W is closely tied to the choice of the auxiliary state $|\phi\rangle$. We expect the algorithm should work for any n -qubit $|a\rangle$. So $|\phi\rangle$ shouldn't be biased toward any n -qubit basis vector, We can choose, e.g.,

$$|\phi\rangle = H^{\otimes n}|0\rangle_n = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle_n$$

where $|\phi\rangle$ is easy to prepare, and almost orthogonal to any $|x\rangle_n$.

As well consider the construction of $-W$

$$-W = 1 - 2|\phi\rangle\langle\phi| = H^{\otimes n}(1 - 2|00\dots 0\rangle\langle 00\dots 0|)H^{\otimes n}$$

Notice that $H^{\otimes n}$ is its own inverse.

Now we need an operation

$W' = 1 - 2|00\dots 0\rangle\langle 00\dots 0|$, which obeys

$$W'|x\rangle_n = \begin{cases} |x\rangle_n & x \neq 00\dots 0 \\ -|x\rangle_n & x = 00\dots 0 \end{cases}$$

One can verify that

$$W' = X^{\otimes n}(C^{n-1}Z)X^{\otimes n}$$

where $C^{n-1}Z$ is the $(n-1)$ -fold controlled- Z gate.

3.3 Performance by Geometrical Analysis

As we discussed in the geometrical picture, each application of WV reduces the angle between the resulting state and $|a\rangle$ by 2θ .

With our choice of $|\phi\rangle$,

$$\cos\left(\frac{\pi}{2} - \theta\right) = \langle a|\phi\rangle = 2^{-n/2} \approx \frac{1}{\sqrt{N}}$$

For large \sqrt{N} , it's fairly accurate that $\theta \approx 2^{-n/2}$. To rotate $|\phi\rangle$ to $|a\rangle$, we can apply an integral number of WV s. A proper choice of the number is as close as possible to

$$\frac{\frac{\pi}{2}}{2\theta} = \frac{\pi}{4} 2^{n/2} \sim \sqrt{N}$$

and the error in angle is no more than $\theta \sim 1/\sqrt{N}$.

If we now measure the input qubits, we have a very high probability to obtain the desired $|a\rangle$. We can repeat the whole procedure a few times to make sure we successfully find $|a\rangle$ in a practical sense.

4. Quantum Supremacy

IX Superconducting Qubits

1. Conductors and Superconductors

1.1 Simple Metals

The tight-binding model in Lab 6 is a good starting point to understand conductors, in particular, metals.

Fermi energy E_F .

the density of states

$$\nu(E) \propto E^{\frac{1}{2}}$$

As a result, the energy dissipation in metals are characterized by a finite resistivity

$$\rho = \frac{m}{ne^2\tau}$$

where τ is the average collision time.

1.2 Superconductivity

From microscopic point of view, the Fermi sea in a metal is unstable under attractive electron-electron interaction mediated by phonons, or lattice vibrations. As a result, electrons with opposite momentum \vec{k} and spin σ pair in k -space are locked into Cooper pairs and form a coherent state

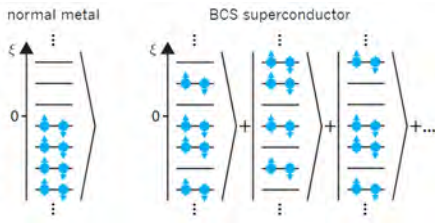


Figure 7: Electrons form a coherent state

The electron pairs can be broken to create a pair of (Bogoliubov) quasiparticles.

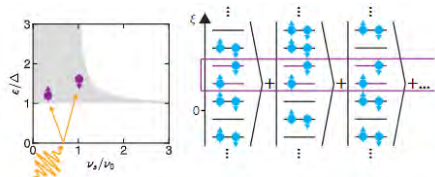


Figure 8: create a pair of quasiparticles

Due to the attractive electron-electron interaction mediated by phonons, this process requires a minimum energy

of 2Δ , where Δ is known as the superconducting gap. For aluminum, this gap is about 1 K.

When temperature is sufficiently low ($k_B T \ll \Delta$), the system condenses into the coherent state, known as the Bardeen-Cooper-Schrieffer (BCS) state.

Only unpaired quasiparticles can be scattered by impurities, hence dissipating energy to the lattice. But their number is exponentially suppressed at low temperatures

$$n_{qp} \sim e^{-\Delta/(k_B T)}$$

according to the Boltzmann distribution.

Therefore, a superconductor can be thought of as a macroscopic quantum state, characterized by the number N_s of superconducting electron pairs.

2. Tunneling Junctions and The Josephson Effect

2.1 Normal-State Tunneling Junction

Consider a tunneling junction, where two normal-state metallic leads are separated by a thin oxide, or a tunnelling barrier. Due to quantum tunnelling electrons can penetrate through the barrier.

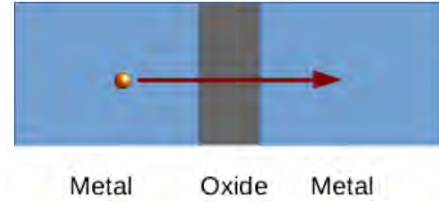


Figure 9: Normal-State Tunneling Junction

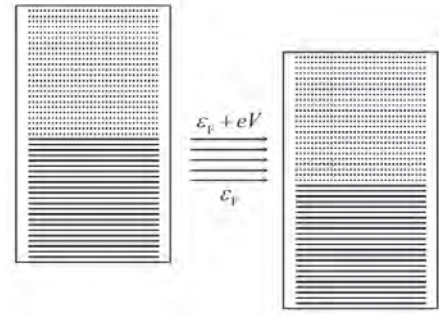


Figure 10: two metals with insulator between

When the Fermi energies on the two sides are shifted by a small voltage bias V (low compared to the barrier

height), electrons in the resulting energy interval eV are able to tunnel from one side to the other without blocking due to the Pauli exclusion principle.

As a result the tunnel current is linear in V and the junction can be characterized as a simple resistor with resistance R_N . One can show

$$G_N = \frac{1}{R_N} \propto \frac{e^2}{h} (\nu_L \nu_R) t^2$$

where t is the energy gain from tunneling, and $\nu_{L,R}$ are the densities of states of the two leads.

2.2 Superconducting Tunneling Junction

When we cool the two metallic leads below their superconducting transition temperature, they become superconducting leads.

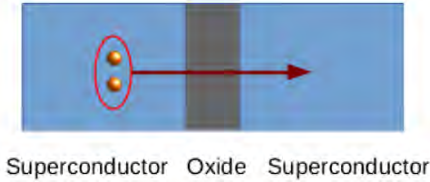


Figure 11: Superconducting Tunneling Junction

Now, dissipation is negligible, and the tunneling resistance is replaced by a non-linear inductor. The physical picture is that quantum wave functions on the two sides overlap with each other in the barrier. Therefore, Cooper pairs can still flow, leading to what is known as the supercurrent (though, on a weaker scale of the order of 10 A/cm²), through the tunneling barrier where the superconducting gap is strongly suppressed (hence, a weak link).

This is a striking manifestation of the quantum nature of superconductivity, known as the Josephson effect. It leads to the only known non-linear non-dissipative circuit element, **the Josephson junction (Josephson 结)**.

2.3 The Josephson Effect

In the limit of low temperatures $k_B T \ll 2\Delta$ and low frequencies $\hbar\omega \ll 2\Delta$, we can model electrons in each lead by a single quantum state $|N\rangle$, labeled by the number of electron pairs. For the two leads connected by a tunnel junction, there is a large family of degenerate ground states $|N_L, N_R\rangle$, labeled by the number of Cooper pairs in the two leads.

Note $N_L + N_R$ is a constant due to charge conservation. We can, alternatively, use $m = (N_R - N_L)/2$ to represent the family of states as

$$|m\rangle \equiv |N_L, N_R\rangle$$

The tunneling of a Cooper pair leads to the change of m by 1, like a particle hopping to an adjacent site on a lattice.

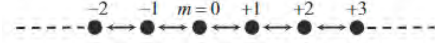


Figure 12: the family of states

Therefore, we consider the phenomenological Hamiltonian

$$\hat{H}_T = -\frac{1}{2} E_J \sum (|m\rangle \langle m+1| + |m+1\rangle \langle m|)$$

where E_J is called the Josephson coupling energy, which is related to the normal-state conductance G_N by the Ambegaokar-Baratoff relation

$$E_J = \frac{\Delta}{2} \frac{h}{(2e)^2} G_N$$

We will find a linear superposition of the degenerate states that diagonalizes \hat{H}_T (i.e., degenerate perturbation) and finding energy eigenvalues, which is first order in E_J .

The eigenstates are

$$|\varphi\rangle = \sum_{m=-\infty}^{+\infty} e^{im\varphi} |m\rangle$$

where φ is like wave vector “ k ”, if we think m as a site.

In the φ representation, a wave function is given by

$$\psi(\varphi) = \langle \varphi | \psi \rangle = \sum_{m=-\infty}^{+\infty} e^{-im\varphi} \langle m | \psi \rangle$$

In an analogy to free electrons, the “momentum” operator is $\hbar\varphi$, and the “position” operator would be

$$\hat{n} \equiv \sum_m |m\rangle m \langle m|$$

Hence,

$$\begin{aligned}
\langle \varphi | (\hat{n} | \psi \rangle) &= \sum_{m=-\infty}^{+\infty} e^{-im\varphi} \langle m | \left(\sum_{m'} |m'\rangle m' \langle m' | \psi \rangle \right) \\
&= \sum_{m=-\infty}^{+\infty} e^{-im\varphi} m \langle m | \psi \rangle \\
&= i \frac{d}{d\varphi} \sum_{m=-\infty}^{+\infty} e^{-im\varphi} \langle m | \psi \rangle \\
&= i \frac{d}{d\varphi} \psi(\varphi)
\end{aligned}$$

Therefore, we find

$$\hat{n} \equiv i \frac{d}{d\varphi}$$

As we work out in Lab 6 for the tight-binding model,

$$H_T |\varphi\rangle = E(\varphi) |\varphi\rangle = -E_J \cos \varphi |\varphi\rangle$$

The “group velocity” would, then, be

$$v_g(\varphi) = \frac{1}{\hbar} \frac{\partial}{\partial \varphi} (-E_J \cos \varphi) = \frac{E_J}{\hbar} \sin \varphi$$

So the net current flowing is given by the **dc Josephson relation**

$$I = (2e)v_g(\varphi) = I_c \sin \varphi$$

where $I_c = \frac{2e}{\hbar} E_J$.

The maximum possible coherent (dissipationless) current I_c occurs at $\varphi = \frac{\pi}{2}$ and is called the **critical current**.

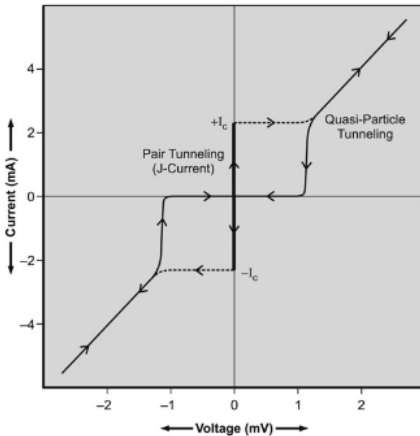


Figure 13: critical current

If more current than this is forced through the junction, the low-energy effective model is no longer applicable.

There is a finite resistance, and the voltage rises from zero to a high value above 2Δ .

We consider the situation where an external electric field is applied and maintained in such a way that there is a fixed voltage drop V across the tunnel junction. This adds to the Hamiltonian a “potential” term $U = -(2e)V\hat{n}$.

The time rate of change of the “momentum” $\hbar\varphi$ to the ‘force’ $2eV$ would be (notice $F = dp/dt$)

$$\hbar \frac{d\varphi}{dt} = -\frac{dU}{d\hat{n}} = 2eV$$

or

$$V = \frac{\hbar}{2e} \frac{d\varphi}{dt}$$

This is known as the **ac Josephson relation**.

Putting the two Josephson relations together, we see that a Josephson junction behaves as an inductor with a nonlinear inductance ($V = L_J \frac{dI}{dt}$)

$$L_J(\varphi) = \frac{\hbar}{2e} \frac{1}{I_c \cos \varphi} = \left(\frac{\hbar}{2e} \right)^2 \frac{1}{E_J \cos \varphi}$$

and an inductive (kinetic) energy

$$E(\varphi) = -E_J \cos \varphi$$

Note that $\frac{dE}{dI} = \frac{dE(\varphi)}{d\varphi} / \frac{dI(\varphi)}{d\varphi} = L_J I$

2.4 Charging Energy

The tunneling of a Cooper pair transfers charge $2e$ from one to the other side of the junction. Due to Coulomb interaction, the junction also has a capacitance C_J .

The energy associated with the transfer of \hat{n} pairs of electrons is

$$\begin{aligned}
U &= \frac{Q^2}{2C} = \frac{(2e)^2}{2C} \hat{n}^2 = 4E_C \hat{n}^2 \\
E_C &= \frac{e^2}{2C}
\end{aligned}$$

In the absence of the additional capacitance, we have, here, $C = C_J$.

3. Superconducting Qubits

We have studied a single isolated Josephson junction which is able to coherently transfer Cooper pairs from one superconducting island to another.

With Coulomb interaction, an artificial atom can be realized and used as a qubit.

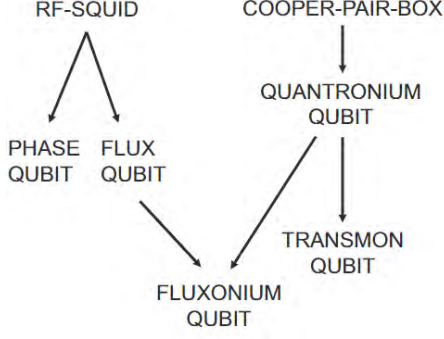


Figure 14: Superconducting Qubit Evolutionary Phylogeny

3.1 The Cooper Pair Box

A Cooper pair box qubit has a voltage source biasing the box through a coupling ('gate') capacitor C_g .

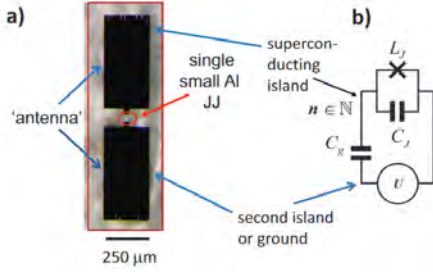


Figure 15: The Cooper Pair Box

The gate capacitor introduces a continuous offset $n_g = -C_g V / (2e)$, whose fluctuations can be overcome in the transmon qubit design.

Except for the n_g term, the Hamiltonian becomes that of a quantum rotor in a gravitational field

$$H = 4E_C(\hat{n} - n_g)^2 - E_J \cos \varphi$$

For small amplitude oscillations, the rotor is roughly a simple harmonic oscillator. This happens in the quantum case in the limit $E_J \gg E_C$, where the zero-point fluctuations in the phase are small.

Up to an irrelevant constant in the energy (and ignoring the offset charge for the moment) we obtain

$$H \approx 4E_C \hat{n}^2 + \frac{1}{2} E_J \hat{\varphi}^2$$

Notice $E_C = e^2 / (2C)$, and $C = C_J + C_g$ is the total capacitance between the two superconducting islands.

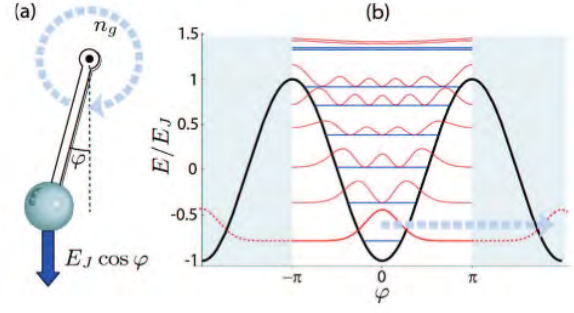


Figure 16: a quantum rotor in a gravitational field

Table 1: The comparison

	Harmonic Oscillator	Cooper Pair Box
Position	x	\hat{n}
Momentum	p	$\hbar \hat{\varphi}$
Kinetic E	$\frac{p^2}{2m}$	$\left(\frac{E_J}{2}\right) \hat{\varphi}^2$
Potential E	$\frac{kx^2}{2}$	$4E_C \hat{n}^2$
Resonant ω	$\sqrt{\frac{k}{m}}$	$\frac{\sqrt{8E_J E_C}}{\hbar}$

The comparison leads to the resonant frequency of the CPB

$$\Omega_J = \frac{1}{\hbar} \sqrt{8E_J E_C}$$

The resonant frequency is also known as the Josephson plasma frequency

$$\Omega_J = \frac{1}{\sqrt{L_J(\varphi=0)C}}$$

$$L_J = \left(\frac{\hbar}{2e}\right)^2 \frac{1}{E_J \cos \varphi}$$

1) The approximation we made replaces the Josephson junction by a linear inductance $L = L_J(\varphi=0)$.

2) The non-linear inductance of the junction will make the energy levels of the Cooper pair box anharmonic.

- Good: Flatter energy levels, insensitive to charge fluctuations
- Bad: Decreasing anharmonicity

3.2 Temperature

The superconducting transition temperature T_c of Al is about 1 K, which can be converted to 21 GHz.

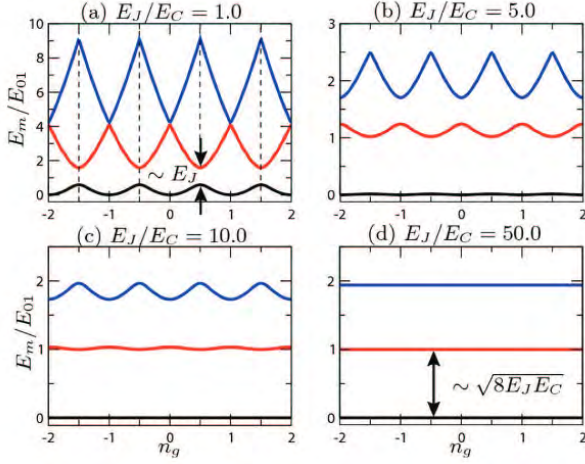


Figure 17: Effects of increasing E_J/E_C

So the operating temperature must satisfy $T \ll T_c$. This is achieved by working inside a dilution refrigerator with base temperature about 30 mK.

The transition frequency of a qubit is usually a few GHz, which is much greater than T , so thermal fluctuations are suppressed. Nevertheless, experiments have found a surprisingly large amount of nonequilibrium quasiparticles that lead to qubit energy relaxation $|1\rangle \rightarrow |0\rangle$.

X Control and Readout of Superconducting Qubits

1. Quantizing the EM Field in a Cavity

1.1 Coupling Atoms to Photons

Quantum electrodynamics (QED) studies atoms and electrons coupled to quantum fluctuations of the electromagnetic (EM) field.

By adjusting the incoming microwave frequency, one can either perform a qubit rotation (at the qubit transition frequency) or a measurement of the state (near the cavity frequency).

1.2 Quantizing the EM Field: Photons

The Hamiltonian (or energy) of the EM field in a cavity is

$$H = \int_V d^3r \left[\frac{1}{2} \epsilon_0 E^2(\vec{r}, t) + \frac{1}{2\mu_0} B^2(\vec{r}, t) \right]$$

According to Maxwell's equations in a cavity, we can, roughly speaking, regard E as x and B as p . This leads to the quantization of the EM field in the cavity: Each mode is a harmonic oscillator. This is not unlike the discrete modes of a musical instrument getting quantized.

To realize such a cavity in circuit QED, one can use a coplanar waveguide (CPW) resonator formed by superconducting wires.

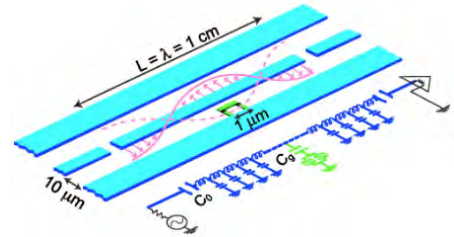


Figure 18: a coplanar waveguide (CPW) resonator

The energy of a single mode with frequency ω_c is

$$E_n = \left(n + \frac{1}{2} \right) \hbar \omega_c$$

In the picture of quantum field, the electric field operator is $\vec{E}_c = \hat{e} E_{c0} (a + a^\dagger)$, where a is the photon annihilation operator and \hat{e} the polarization direction.

Recall that the operators obey

- $[a, a^\dagger] \equiv aa^\dagger - a^\dagger a = 1$
- With $N = a^\dagger a$, $[a, N] = a$ and $[a^\dagger, N] = -a^\dagger$

We usually choose the eigenstates $|n\rangle$ of N to be the basis.

- $N|n\rangle = n|n\rangle$
- $a|n\rangle = \sqrt{n}|n-1\rangle$, where $\langle n|n\rangle = 1$

In the number basis, it is rather easy to calculate matrix elements. The elementary ones are $\langle n-1|a|n\rangle = \sqrt{n}$ and $\langle n+1|a^\dagger|n\rangle = \sqrt{n+1}$.

Alternatively, we can write

$$a = \sum_n \sqrt{n+1} |n\rangle \langle n+1|$$

$$a^\dagger = \sum_n \sqrt{n+1} |n+1\rangle \langle n|$$

We can now associate the constant in the field operator

$$E_{c0} \equiv \sqrt{\langle 0|E_c^2|0\rangle} = \sqrt{\langle 0|E_{c0}a|1\rangle \langle 1|E_{c0}a^\dagger|0\rangle}$$

with vacuum fluctuations (through virtual photon emission and reabsorption) in the vacuum $|0\rangle$.

Meanwhile, the energy due to vacuum fluctuations is

$$\frac{\hbar\omega}{2} = 2V_c \left[\frac{\epsilon_0 \langle 0|E_c^2|0\rangle}{2} \right]$$

where V_c is the volume of the cavity and the factor of 2 takes care of the coexisting magnetic field energy. So,

$$E_{c0} = \sqrt{\langle 0|E_c^2|0\rangle} = \sqrt{\frac{\hbar\omega_c}{2\epsilon_0 V_c}}$$

One can conclude that a small cavity enhances quantum fluctuations of the electric field.

2. Coupling Between Atom and EM Field

With the quantized field, we can establish a fully quantum-mechanical model to describe the interaction between qubits and photons.

The Jaynes-Cummings model has a Hamiltonian

$$H_{JC} = \underbrace{-\frac{1}{2}\hbar\omega_{01}\sigma_z}_{H_{qubit}} + \underbrace{\hbar\omega_c \left(a^\dagger a + \frac{1}{2} \right)}_{H_{field}} + \underbrace{\hbar g(a\sigma_+ + a^\dagger\sigma_-)}_{H_{int}}$$

where $\sigma_\pm = \frac{\sigma_x \pm i\sigma_y}{2}$. Notice that $\sigma_+|g\rangle = |e\rangle$, $\sigma_-|e\rangle = |g\rangle$ and $\sigma_+|e\rangle = \sigma_-|g\rangle = 0$.

The quantum Hamiltonian arises from a coupling between the electric field \vec{E} in a single-mode cavity and the dipole moment \vec{p} of the artificial atom at position \vec{R} given by

$$U = -\vec{p} \cdot \vec{E}(\vec{R})$$

This dipole moment connects the ground and excited state of the atom, and the interaction term reads

$$H_{int} = -|e\rangle \langle e| \vec{p} \cdot \vec{E}(\vec{R}) |g\rangle \langle g| + h.c.$$

$$= \hbar g(a + a^\dagger)\sigma_x$$

where the vacuum Rabi coupling

$$g = -\langle e|\vec{p} \cdot \hat{e}|g\rangle \frac{E_{c0}}{\hbar}$$

The interaction can be rewritten as

$$H_{int} = \hbar g(a + a^\dagger)(\sigma_+ + \sigma_-)$$

$$= \hbar g(a\sigma_+ + a^\dagger\sigma_-) + \hbar g(a\sigma_- + a^\dagger\sigma_+)$$

If the cavity mode is close in frequency to the qubit transition frequency, the first term is important because it nearly conserves the total energy.

The second term mixing states that are far away from each other is often dropped in the so-called **rotating wave approximation**.

We arrive at the Jaynes-Cummings Hamiltonian, which may further include external driving and damping terms.

2.1 Solving the JC Hamiltonian

The Hilbert space is the tensor product of a harmonic oscillator and a qubit, whose basis vectors are

$$|0, g\rangle, |1, g\rangle, |2, g\rangle, \dots$$

$$|0, e\rangle, |1, e\rangle, |2, e\rangle, \dots$$

where the first index is the number of photons and the second the qubit state ($g \equiv 0, e \equiv 1$). (详细见 lab8)

The first two terms in H_{JC} is already diagonal, i.e.,

$$\langle n, \sigma | H_{qubit} + H_{field} | m, \sigma' \rangle = (\hbar\omega_{01}\sigma + n\hbar\omega_c)\delta_{nm}\delta_{\sigma\sigma'}$$

up to an unimportant constant.

To be exact, we need infinitely many basis states. However, when the temperature is low and when we are

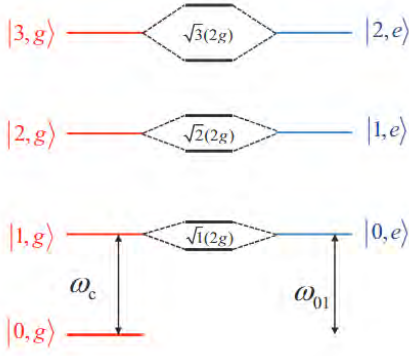


Figure 19: a harmonic oscillator and a qubit

not interested in pumping in more than a few photons, we can truncate the Hilbert space to include just a few basis states (in the absence of qubit-cavity interaction).

Let us consider the case where the detuning between the qubit and cavity frequencies

$$\Delta \equiv \omega_{01} - \omega_c = 0$$

Photon and qubit excitations hybrid into the so-called polaritons.

In the case $\Delta = 0$, the two states $|n+1, g\rangle$ and $|n, e\rangle$ are degenerate in the absence of interaction.

The dipole coupling lift the degeneracy by introducing off-diagonal matrix elements (which are real)

$$\langle n+1, g | H_{int} | n, e \rangle = \langle n, e | H_{int} | n+1, g \rangle = \sqrt{n+1} \hbar g$$

In the truncated 2D subspace, the effective Hamiltonian is

$$\begin{aligned} H' &= \begin{pmatrix} (n+1)\hbar\omega_c & \sqrt{n+1}\hbar g \\ \sqrt{n+1}\hbar g & (n+1)\hbar\omega_c \end{pmatrix} \\ &= (n+1)\hbar\omega_c I_{2 \times 2} + \sqrt{n+1}\hbar g \sigma_x \end{aligned}$$

The energy eigenstates are coherent superpositions

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}}(|n+1, g\rangle \pm |n, e\rangle)$$

i.e., the bonding-anti-bonding combination of photon and qubit excitation, known as polaritons.

The corresponding energies are

$$E_{\pm} = (n+1)\hbar\omega_c \pm \sqrt{n+1}\hbar g$$

In this approximation, we have neglect the coupling of the levels to those with energy difference $2\hbar\omega_c$, due to the second term of the interaction (see Lab for explanation).

In the so-called dispersive regime, where $|\Delta| \gg g$, the truncated Hamiltonian becomes

$$\begin{aligned} H' &= \begin{pmatrix} (n+1)\hbar\omega_c & \sqrt{n+1}\hbar g \\ \sqrt{n+1}\hbar g & n\hbar\omega_c + \hbar\omega_{01} \end{pmatrix} \\ &= \epsilon_n I_{2 \times 2} + \sqrt{n+1}\hbar g \sigma_x - \frac{\hbar\Delta}{2} \sigma_z \end{aligned}$$

where

$$\epsilon_n = \left(n + \frac{1}{2}\right) \hbar\omega_c + \frac{1}{2} \hbar\omega_{01}$$

One can verify that H' reduces to the degenerate form when $\Delta \equiv \omega_{01} - \omega_c = 0$

Up to a constant, the Hamiltonian represents a spin in a pseudo magnetic field $\vec{B} = (\sqrt{n+1}\hbar g, 0, \frac{\Delta}{2})$. Just like in a Stern-Gerlach measurement, the eigenenergies can be obtained as

$$E_{\pm} = \epsilon_n \pm |\vec{B}| = \epsilon_n \pm \frac{\hbar\Delta}{2} \sqrt{1 + \frac{4g^2}{\Delta^2}(n+1)}$$

In the dispersive limit ($|\Delta| \gg g$) we can perform a Taylor series expansion

$$E_{\pm} = \epsilon_n \pm \frac{\hbar\Delta}{2} \left[1 + \frac{1}{2} \frac{4g^2}{\Delta^2}(n+1) + O\left(\frac{g^4}{\Delta^4}\right) \right]$$

Comparing to the uncoupled system

$$\begin{aligned} \Delta E_{n+1,g} &= -\hbar \frac{g^2}{\Delta}(n+1) = -\hbar \frac{g^2}{\Delta} \left[(n+1) + \frac{1}{2} \right] + \hbar \frac{g^2}{\Delta} \\ \Delta E_{n,g} &= \hbar \frac{g^2}{\Delta}(n+1) = \hbar \frac{g^2}{\Delta} \left(n + \frac{1}{2} \right) + \hbar \frac{g^2}{\Delta} \end{aligned}$$

The coupling introduces an effective potential, up to a constant

$$V_{dispersive} = -\hbar \frac{g^2}{\Delta} \left[a^\dagger a + \frac{1}{2} \right] \sigma_z$$

in the limit of $g \rightarrow 0$.

This is result of a second-order perturbation. It can be interpreted as a shift in the cavity frequency which depends on the state of the qubit, thus can be measured without directly disturbing the qubit state.

3. Two Qubits Coupled Through a Cavity

Two qubits connected to the same resonator can be coupled passively through its virtual excitations.

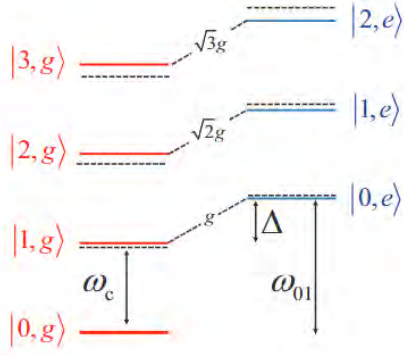


Figure 20: the result of a second-order perturbation

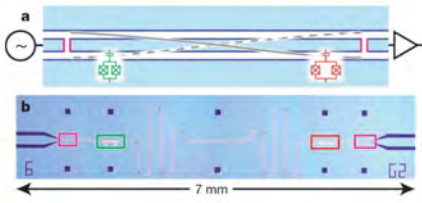


Figure 21: Two Qubits Coupled Through a Cavity

The effective Hamiltonian for the resonator and two such qubits can be obtained as

$$\begin{aligned}
 H_{12}^{eff} = & \left[\hbar\omega_c \left(a^\dagger a + \frac{1}{2} \right) \right]_{field} - \left[\frac{\hbar\omega_{01}}{2} (\sigma_{1z} + \sigma_{2z}) \right]_{qubits} \\
 & - \frac{\hbar g^2}{\Delta} \left(a^\dagger a + \frac{1}{2} \right) (\sigma_{1z} + \sigma_{2z}) \\
 & - \frac{\hbar g^2}{\Delta} (\sigma_{1+}\sigma_{2-} + \sigma_{1-}\sigma_{2+})
 \end{aligned}$$

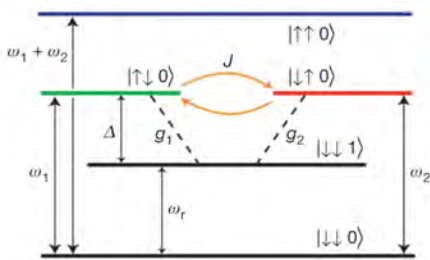


Figure 22: the state of the resonator mode

The qubits should be tuned in resonance with each other, but away from the resonator's frequency.

In the qubit subspace

$$U(t) = e^{i \frac{\hbar g^2}{\Delta} (a^\dagger a + \frac{1}{2}) (\sigma_{1z} + \sigma_{2z})}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \frac{g^2}{\Delta} t & i \sin \frac{g^2}{\Delta} t & 0 \\ 0 & i \sin \frac{g^2}{\Delta} t & \cos \frac{g^2}{\Delta} t & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

This does not change the state of the resonator mode. At $t = \frac{\pi |\Delta|}{4g^2}$, it corresponds to a $\sqrt{i}SWAP$ operation.

XI Noise, General Measurement, and Qubit Decoherence

1. Classes of Errors in a Circuit Model

- 1) State preparation. Need to couple qubits to other items (cavities, controls, measurement devices) and apply complex protocols to ensure a fast reset.
- 2) Gate imperfection. Imprecise amplitude, phase, or duration of microwave pulses, and qubit frequency fluctuations.
- 3) Measurement errors. Limited integration time, measurement induced decoherence, and amplifier and detector noise.
- 4) Qubit decoherence. Environment induced relaxation, heating, and dephasing, as well as crosstalk, unwanted interaction between the qubits.

2. Insights from Classical Noise

We can model the single-stage process by a probability p for the bit to flip, and a probability $1 - p$ for the bit to remain the same.

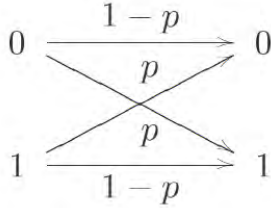


Figure 23: single-stage process

Therefore, a classical state is described by a vector of probabilities. We only need to know the evolution matrix (or matrix of transition probabilities), which states that

$$p(Y = y) = \sum_x p(Y = y|X = x)p(X = x)$$

The previous example can be expressed in a matrix form as

$$\begin{bmatrix} p(Y = 0) \\ p(Y = 1) \end{bmatrix} = \begin{pmatrix} 1-p & p \\ p & 1-p \end{pmatrix} \begin{bmatrix} p(X = 0) \\ p(X = 1) \end{bmatrix}$$

or, in a short notation

$$\vec{p}_Y = E\vec{p}_X \equiv \mathcal{E}(\vec{p}_X)$$

The evolution matrix E requires

- 1) all the entries of E must be non-negative; the positivity condition resulting in positive probabilities only,

- 2) all the columns of E must sum to one; the completeness condition resulting in conserved total probability.

To model these effects, we use the density matrix language to describe probabilistic quantum states and study their evolution in the presence of an environment.

3. Quantum Operation Formalism

3.1 Density Matrices and Quantum Operations

Quantum systems are inherently probabilistic. Measurements or random perturbations lead to probabilistic outcomes, which are described in terms of density matrices.

For example, to prepare a quantum state $|\psi\rangle$, a noisy quantum system likely produces a random distribution of quantum states, i.e., $|\psi_i\rangle$ with probability p_i , due to imprecise controls or environmental noise. We use the density matrix

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$$

to describe the mixed state, as oppose to $p_0 = |\psi\rangle \langle \psi|$.

The quantum operation formalism is a general tool for describing the evolution of quantum systems. Similar to how classical states evolves, quantum states transform as

$$\rho' = \mathcal{E}(\rho)$$

The map \mathcal{E} in this equation is a **quantum operation**.

The dynamics of a closed quantum system are described by a unitary transform. An unitary evolution is a quantum operation:

$$\mathcal{E}(\rho) = U\rho U^\dagger$$

which results from $|\psi'_i\rangle = U|\psi_i\rangle$.

On the other hand, measurement is also a quantum operation. However, the process of measurement is irreversible and probabilistic.

For the computational basis (projective) measurement, we take $M_1 = |0\rangle \langle 0|$ and $M_2 = |1\rangle \langle 1|$. If the initial state is $|\psi_i\rangle$, we obtain the outcome m with probability

$$p_i^m = |\langle m|\psi_i\rangle|^2 = |M_m|\psi_i\rangle|^2 = \langle \psi_i|M_m^\dagger M_m|\psi_i\rangle$$

and the state after the measurement is

$$|\psi_i^m\rangle = \frac{M_m|\psi_i\rangle}{|M_m|\psi_i\rangle|} = \frac{M_m|\psi_i\rangle}{\sqrt{\langle \psi_i|M_m^\dagger M_m|\psi_i\rangle}}$$

The total probability of obtaining m is

$$\begin{aligned}\rho_m &= \sum_i p_i p_i^m = \sum_i p_i \langle \psi_i | M_m^\dagger M_m | \psi_i \rangle \\ &= \sum_i p_i \text{Tr}(M_m^\dagger M_m | \psi_i \rangle \langle \psi_i |) \\ &= \text{Tr}(M_m^\dagger M_m \rho) = \text{Tr}(M_m \rho M_m^\dagger)\end{aligned}$$

Similarly, the density matrix of the resulting state is

$$\begin{aligned}\rho' \equiv \mathcal{E}(\rho) &= \sum_i p_i \left[\sum_m p_i^m | \psi_i^m \rangle \langle \psi_i^m | \right] \\ &= \sum_m M_m \rho M_m^\dagger\end{aligned}$$

So far, we have shown that the quantum operation formalism is a general tool for describing the evolution of quantum systems, including unitary transformations $\mathcal{E} = U\rho U^\dagger$ and measurements $\mathcal{E}(\rho) = M_m \rho M_m^\dagger$.

We can now develop a general theory of quantum operations, motivated by the physical reality of a system coupled to an environment.

As one can anticipate from the previous discussions on unitary transformations and measurements, quantum operations can be represented in an elegant **operator-sum representation**.

3.2 Operator-Sum Representation

Assume the system S is part of a larger and closed system, which also includes the environment E . For practical interest, we can assume the initial density matrix is separable

$$\rho = \rho_S(0) \otimes \rho_E(0)$$

where $\rho_E(0) |e_0\rangle \langle e_0|$ is a pure state. Let $|e_k\rangle$ be orthonormal basis for the environmental state space.

The system and the environment are coupled by a time-independent Hamiltonian H , leading to a unitary time evolution of the total system.

We then take a partial trace over the environment, which allows us to obtain the reduced state of the system alone.

As illustrated in the figure, the partial trace can be represented by a measurement in $|e_k\rangle$ basis of the environment (qubits). However, we do not acquire the outcome k from the measurement.

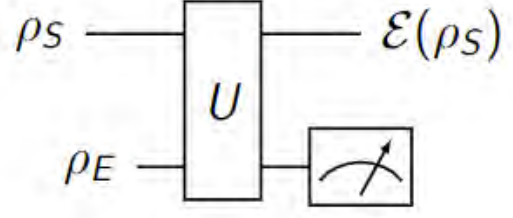


Figure 24: a partial trace over the environment

Put together, with the time evolution operator $U(t) = e^{iHt/\hbar}$, the evolution of the reduced density matrix (which we care) is

$$\begin{aligned}\rho_S(t) &= \text{Tr}_E \{ U(t) [\rho_S(0) \otimes |e_0\rangle \langle e_0|] U^\dagger(t) \} \\ &= \sum_k \langle e_k | U(t) | e_0 \rangle \rho_S(0) \langle e_0 | U^\dagger(t) | e_k \rangle \\ &= \sum_k E_k \rho_S(0) E_k^\dagger\end{aligned}$$

where $E_k = \langle e_k | U(t) | e_0 \rangle$ are known as the **Kraus operator** acting on the Hilbert space of the system.

The Kraus operators satisfy the completeness constraint $\sum_k E_k^\dagger E_k = 1$, if no information about what occurred in the process is obtained by measurement.

The Kraus operators encode all the available information about the initial state of the environment and about the dynamics of the system-environment coupling. Therefore, the operator-sum representation describes the dynamics of the system without having to explicitly consider properties of the environment.

Consequently, the reduced density matrix of the system satisfies:

- $\rho_S(t)$ is Hermitian.
- $\rho_S(t)$ has unit trace.
- $\rho_S(t)$ is positive.

These properties can be compared to the positivity and completeness conditions in the description of classical noise.

In general, the evolution is not unitary, and $\rho_S(t)$ is in a mixed state after partial trace. There is an arrow of time, i.e., E_k are not invertible.

3.3 General Measurements

The structure of the operator-sum representation is similar to the quantum operation of projective measure-

ment

$$\mathcal{E}_m(\rho) = \sum_m M_m \rho M_m^\dagger$$

where $P_m \equiv M_m = M_m^\dagger$ is a projector. This allows us to interpret $\{E_k\}$ as a general measurement of the qubit system, with a projective measurement $I^S \otimes P_k^E$ on the composite system.

The quantum operation takes the state ρ_S and randomly replaces it by

$$\rho_k = \frac{E_k \rho E_k^\dagger}{\text{Tr}(E_k \rho E_k^\dagger)}$$

with probability $\text{Tr}(E_k \rho E_k^\dagger)$. The result of ρ_k is the direct consequence of the outcome k from the measurement of the environment.

In theoretical study, projective measurements are usually enough because most physical system can only be measured in a very coarse manner.

In qubit readouts, however, we aim for an exquisite level of control over the measurements that can be done. Such a real measurement involves an ancilla system (i.e., an environment); in the qubit-cavity case, it is the cavity.

Therefore, we need to consider, in general, the unitary evolution of the composite quantum system and the measurement of the ancilla system. The index k labels the readout of the ancilla system.

4. Qubit Decoherence

In general, superconducting qubits are not identical and contains (magnetic) impurities and quasiparticle excitations, hence are subject to various random sources of noise.

The effects of noise are usually separated into two terms:

- Relaxation: transition that change the qubit state.
- Dephasing: modulation of transition frequencies which leads to phase randomization.

4.1 Amplitude Damping

The amplitude-damping channel is a schematic model of the decay of an excited state of a qubit due to spontaneous emission of a photon.

We denote the qubit ground state by $|g\rangle$ and the excited state of interest by $|e\rangle$. The “environment” is the

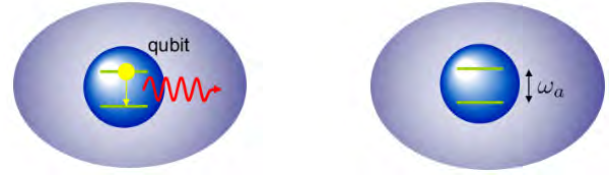


Figure 25: The effects of noise

electromagnetic field, assumed initially to be in its vacuum state $|0\rangle$. After a while, there is a probability p that the excited state has decayed to the ground state and a photon has been emitted, so that the environment has made a transition from the state $|0\rangle$ (“no photon”) to the state $|1\rangle$ (“one photon”).

The unitary evolution U_{SE} of the qubit and environment is

$$\begin{aligned} |g\rangle |0\rangle &\rightarrow |g\rangle |0\rangle \\ |e\rangle |0\rangle &\rightarrow \sqrt{1-p} |e\rangle |0\rangle + \sqrt{p} |g\rangle |1\rangle \end{aligned}$$

By evaluating the partial trace over the environment, we find the Kraus operators

$$\begin{aligned} E_0 &= \langle 0 | U_{SE} | 0 \rangle = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix} \\ E_1 &= \langle 1 | U_{SE} | 0 \rangle = \begin{pmatrix} 0 & p \\ 0 & 0 \end{pmatrix} \end{aligned}$$

The density matrix evolves as

$$\begin{aligned} \rho_S(0) &= \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} \\ \rho_S(t) &= E_0 \rho_S(0) E_0^\dagger + E_1 \rho_S(0) E_1^\dagger \\ &= \begin{pmatrix} \rho_{gg} & \sqrt{1-p} \rho_{ge} \\ \sqrt{1-p} \rho_{eg} & (1-p) \rho_{ee} \end{pmatrix} + \begin{pmatrix} p \rho_{ee} & 0 \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \rho_{gg} + p \rho_{ee} & \sqrt{1-p} \rho_{ge} \\ \sqrt{1-p} \rho_{eg} & (1-p) \rho_{ee} \end{pmatrix} \end{aligned}$$

If we apply the channel n times in succession, we have

$$\rho_{ee} \rightarrow (1-p) \rho_{ee} \rightarrow (1-p)^2 \rho_{ee} \rightarrow \cdots \rightarrow (1-p)^n \rho_{ee}$$

Introducing a **relaxation time** T_1 , we can identify the $|e\rangle \rightarrow |g\rangle$ transition probability in given $\delta t \ll T_1$ as $p = \frac{\delta t}{T_1} \approx 1 - e^{-\delta t/T_1}$. The probability that the excited state persists for time t is

$$P(t) = (1-p)^{t/\delta t} \approx e^{-t/T_1}$$

As $t \rightarrow \infty$, the reduced density matrix approaches

$$\lim_{t \rightarrow \infty} \rho_S(t) = \begin{pmatrix} \rho_{gg} + \rho_{ee} & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

So, due to spontaneous emission, the qubit always ends up in its ground state. The coherence between $|g\rangle$ and $|e\rangle$ is also lost (but at half the rate).

4.2 Phase Damping

Phase damping can be modeled as a Brownian motion of the phase, which accumulates random displacements due to the fluctuation in the qubit energy levels.

The operator-sum description of this quantum process reads

$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-q} \end{pmatrix}$$

$$E_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{q} \end{pmatrix}$$

The density matrix evolves as

$$\begin{aligned} \rho_S(t) &= E_0 \rho_S(0) E_0^\dagger + E_1 \rho_S(0) E_1^\dagger \\ &= \begin{pmatrix} \rho_{gg} & \sqrt{1-q} \rho_{ge} \\ \sqrt{1-q} \rho_{eg} & (1-q) \rho_{ee} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & q \rho_{ee} \end{pmatrix} \\ &= \begin{pmatrix} \rho_{gg} & \sqrt{1-q} \rho_{ge} \\ \sqrt{1-q} \rho_{eg} & \rho_{ee} \end{pmatrix} \end{aligned}$$

Unlike amplitude damping, phase damping leads to a pure decay of the off-diagonal elements of the density matrix. We can identify $\sqrt{1-q}$ as $e^{-\delta t/T_\phi}$ in time interval δt , where T_ϕ is known as the pure **dephasing time**.

Alternatively, we can write

$$\rho_S(t) = \sqrt{1-q} \begin{pmatrix} \rho_{gg} & \rho_{ge} \\ \rho_{eg} & \rho_{ee} \end{pmatrix} + (1 - \sqrt{1-q}) \begin{pmatrix} \rho_{gg} & 0 \\ 0 & \rho_{ee} \end{pmatrix}$$

It is as if the qubit were being slightly measured (for small δt , hence $q \ll 1$), continuously in time.

Eventually, the system collapses into a fixed point, $\rho_\infty = \rho_{gg} |0\rangle\langle 0| + \rho_{ee} |1\rangle\langle 1|$, which is a statistical mixture of $|0\rangle$ and $|1\rangle$, with probabilities that reflect the original state amplitudes.

If an experiment combines relaxation ($1-p = e^{-\delta t/T_1}$) and dephasing ($\sqrt{1-q} = e^{-\delta t/T_\phi}$), the relaxation rate $\gamma = \frac{1}{T_1}$ remains the same, but the dephasing rate increases to

$$\frac{1}{T_2^*} = \frac{1}{2T_1} + \frac{1}{T_\phi}$$

Techniques, such as **spin echo**, exist that can suppress phase damping by introducing spin flips during the experiment, such that quasistatic fluctuations can be cancelled. So qubit relaxation, which scrambles the basis states, is the worse type of decoherence.

XII Quantum Error Correction

1. Error Representation and Correction

Errors for a single qubit can be represented by unexpected Z, X , and Y gates (phase error, bit-flip error, and combined bit-flip and phase error, respectively) in a quantum circuit.

Redundancy in coding can reduce the error rate from $p \ll 1$ to $O(p^2)$. The key in quantum error correction lies in how to replicate and extract the information.

1.1 Representation of Errors

Interaction with the environment will transform and entangle the states of the qubit and its environment. In general, we expect the following process:

$$\begin{aligned} |e_0\rangle |0\rangle &\rightarrow |e_1\rangle |0\rangle + |e_2\rangle |1\rangle \\ |e_0\rangle |1\rangle &\rightarrow |e_3\rangle |0\rangle + |e_4\rangle |1\rangle \end{aligned}$$

where $|e_{0-4}\rangle$ are the states of the environment.

For practical quantum computing, we expect weak coupling between the qubit and its environment. Hence we expect

$$\begin{aligned} \sqrt{|\langle e_0|e_1\rangle|^2} &\approx \sqrt{|\langle e_0|e_4\rangle|^2} \approx 1 \\ \langle e_2|e_2\rangle, \langle e_3|e_3\rangle &\ll 1 \end{aligned}$$

To discuss the interaction with the environment, it is useful to rewrite projection operators, which satisfy

$$P_0 |\psi\rangle = |0\rangle \langle 0|\psi\rangle, \quad P_1 |\psi\rangle = |1\rangle \langle 1|\psi\rangle$$

as

$$P_\alpha = \frac{I + (-1)^\alpha Z}{2}$$

We can now write

$$|e_0\rangle |\psi\rangle \rightarrow [|e_1\rangle I + |e_2\rangle X] P_0 |\psi\rangle + [|e_3\rangle X + |e_4\rangle I] P_1 |\psi\rangle$$

where $|e\rangle O |\psi\rangle \equiv |e\rangle \otimes O |\psi\rangle$.

Plugging in the explicit form of P_α , we find

$$\begin{aligned} |e_0\rangle |\psi\rangle &\rightarrow \left[\frac{|e_1\rangle + |e_4\rangle}{2} I + \frac{|e_1\rangle - |e_4\rangle}{2} Z \right. \\ &\quad \left. + \frac{|e_3\rangle + |e_2\rangle}{2} X + \frac{|e_3\rangle - |e_2\rangle}{2} Y \right] |\psi\rangle \\ &\equiv (|d\rangle I + |a\rangle X + |b\rangle Y + |c\rangle Z) |\psi\rangle \end{aligned}$$

The four operators I, Z, X and Y correspond to no error, phase error, bit-flip error, and combined bit-flip and phase error, respectively.

We notice that

$$|d\rangle = \frac{|e_1\rangle + |e_4\rangle}{2} \approx |e_0\rangle$$

but $|a\rangle$, $|b\rangle$, and $|c\rangle$, which are associated with various errors, are ket-vectors with small amplitudes. This is consistent with our weak-coupling assumption. For one qubit, there are 3 terms of errors.

When we generalize the result to 1-bit errors for n -bit codewords $|\Psi_n\rangle$, we can write

$$\begin{aligned} |e_0\rangle |\Psi_n\rangle &\rightarrow |d\rangle |\Psi_n\rangle + \\ &\sum_{i=1}^n (|a_i\rangle X_i |\Psi_n\rangle + |b_i\rangle Y_i |\Psi_n\rangle + |c_i\rangle Z_i |\Psi_n\rangle) \end{aligned}$$

Altogether, there are $(3n + 1)$ terms.

1.2 Error Correction

A classical code is defined as being a set of bit strings with certain properties.

Before 1995, it was believed that the concept of error correction could not apply to quantum systems, for the following reasons:

- 1) Quantum states collapse when measured.
- 2) Errors are continuous.
- 3) Quantum states cannot be cloned.

It turns out there are ways around all of these objections.

- 1) The part of the Hilbert space containing the quantum information to be preserved need not be measured; only the effect of the environment need be determined by a measurement.
- 2) Using entangled states allow errors to be made orthogonal and distinguishable.
- 3) Entanglement also replaces the role played by redundant copies in classical error correction.

To encode each logic qubit in multiple physical qubit, we replace $|0\rangle$ and $|1\rangle$ by the codewords, e.g.

$$\begin{aligned} |\tilde{0}\rangle &= |0\rangle |0\rangle |0\rangle = |000\rangle \\ |\tilde{1}\rangle &= |1\rangle |1\rangle |1\rangle = |111\rangle \end{aligned}$$

One (or two) bit flip moves the states to the non-encoding space $|001\rangle, |010\rangle, |100\rangle, |110\rangle, |101\rangle, |011\rangle$, therefore can

be detected. But as measurement can alter a state, one must come up with less obvious form of measurement.

In addition to bit-flip errors, there can also be phase errors, e.g.

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}} \rightarrow \frac{|0\rangle - |1\rangle}{\sqrt{2}}$$

A generalization of the 3-bit coding to 9-bit can correct both bit-flip and phase errors. See, e.g., D. Gottesman, arXiv:0904.2557, Sec. 2.1.

2. The 3-Bit Repetition Code

While measurement can alter a state, there exist less obvious forms of measurement for error detection. In a repetition code, one can use CNOT gates to extract the information without directly measuring the qubits.

Errors, in general, leads to information leakage into the non-encoding space. One can correct the errors by returning to the encoding space without revealing any information of the logical qubit.

Preparation

$$|\psi\rangle \equiv \alpha |000\rangle + \beta |111\rangle$$

Occasionally, a bit is flipped (with a small probability p).

$$|\psi_1\rangle = X_1 |\psi\rangle = \alpha |100\rangle + \beta |011\rangle$$

$$|\psi_2\rangle = X_2 |\psi\rangle = \alpha |010\rangle + \beta |101\rangle$$

$$|\psi_3\rangle = X_3 |\psi\rangle = \alpha |001\rangle + \beta |110\rangle$$

Detection: We cannot measure the three qubits, but can use CNOT gates to extract the information.

In addition to detection, we can directly correct the error by the following circuit without measuring.

The essence is that we can restore $|\psi\rangle$ without revealing any information about α and β .

3. Toward Fault-Tolerant Quantum Computation

Provided the noise in individual quantum gates is below a certain constant threshold, it is possible to reliably perform an arbitrary quantum computation.

In the modern surface code, errors are allowed to exist and propagate (hence fault-tolerant), as long as they are sparse. Once identified, classical control software can be used to track and correct the errors separately.

3.1 Fault-Tolerant Quantum Computation

Even though the repetition code cannot correct all possible errors, it convinces us that noise is not a serious problem in principle; error correction can reduce the error probability from p to $O(p^2)$.

If we further introduce hierarchical procedures, the error probability can be ultimately reduced to as low a level as desired, as long as the original error rate p is below some threshold p_{th} (with physically reasonable assumptions).

This is known as the threshold theorem, as was also important for early-day classical computation.

3.2 Understanding Error Detection

To understand the connection between error detection and operator measurement, we digress to the following circuit for measurement of an operator U acting on a single qubit.

Here, we suppose U has eigenvalues ± 1 and corresponding eigenvector $|u_{\pm}\rangle$. So a single-qubit state $|\psi\rangle$ can be generically expressed as $\alpha |u_+\rangle + \beta |u_-\rangle$.

Following the circuit from left to right, the two-qubit state evolves as

$$1$$

When the measurement result is 0, the circuit outputs $|u_+\rangle$. Otherwise, it outputs $|u_-\rangle$.

As an example of the circuit that can be used to measure a single-qubit operator U , we consider $U \equiv Z$.

This implies that we can alternatively interpret the repetition code as measuring the product of Z -gates operating on the encoded qubits.

For that reason, let us define

$$U_1 = Z_1 Z_2, \quad U_2 = Z_2 Z_3$$

In fact, an equivalent circuit for error detection, which incorporates U_1 and U_2 explicitly, can be constructed.

The operators U_1 and U_2 each has two distinct eigenvalues ± 1 . The measurement of the operators, for zero and one-qubit errors, yields

Therefore, the measurement results contain the identical information as the measurement of $|x\rangle$ and $|y\rangle$. They are known as the **syndrome**, which can be used to identify and locate errors.

3.3 Toward Fault-Tolerance with the Surface Code

In a surface code, qubits form a two-dimensional array. They are entangled into a randomly selected quiescent state resulting from the measurement of stabilizers.

XIII Review and Outlook

1. DiVincenzo's Criteria

- 1) Well defined extendible qubit array-stable memory
 - 2) Preparable in the “000...” state
 - 3) Single-quantum measurements
 - 4) Universal set of gate operations
 - 5) Long decoherence time ($> 10^4$ operation time)
- And, for quantum communications,
- 6) Interconvert stationary and flying qubits
 - 7) Transmit flying qubits from place to place

1.1 Qubits: The Building Blocks

Qubits are physical carriers of quantum information.

To encode a logic qubit in multiple physical qubit, we replace $|0\rangle$ and $|1\rangle$ by the codewords, e.g., in the 3-qubit repetition code,

$$|\tilde{0}\rangle = |0\rangle|0\rangle|0\rangle = |000\rangle, \quad |\tilde{1}\rangle = |1\rangle|1\rangle|1\rangle = |111\rangle$$

In the 2D complex vector space, any Hermitian operator $\hat{n} \cdot \vec{\sigma}$, where \hat{n} can be expressed as

$$\hat{O} = d\hat{I} + a\hat{\sigma}_x + b\hat{\sigma}_y + c\hat{\sigma}_z$$

where $a, b, c, d \in \mathbb{R}$.

Pauli matrices $\hat{\sigma}_{x,y,z}$ satisfy the following relations:

$$\begin{aligned} \hat{\sigma}_x^2 &= \hat{\sigma}_y^2 = \hat{\sigma}_z^2 = 1 \\ \hat{\sigma}_x \hat{\sigma}_y &= -\hat{\sigma}_y \hat{\sigma}_x = i\hat{\sigma}_z \\ \hat{\sigma}_y \hat{\sigma}_z &= -\hat{\sigma}_z \hat{\sigma}_y = i\hat{\sigma}_x \\ \hat{\sigma}_z \hat{\sigma}_x &= -\hat{\sigma}_x \hat{\sigma}_z = i\hat{\sigma}_y \end{aligned}$$

We can further define

$$\hat{\sigma}_+ = \frac{\hat{\sigma}_x + i\hat{\sigma}_y}{2}, \quad \hat{\sigma}_- = \frac{\hat{\sigma}_x - i\hat{\sigma}_y}{2}$$

Therefore, we have

$$\begin{aligned} \hat{\sigma}_z |g\rangle &= |g\rangle, \quad \hat{\sigma}_z |e\rangle = -|e\rangle \\ \hat{\sigma}_+ |g\rangle &= |e\rangle, \quad \hat{\sigma}_- |e\rangle = |g\rangle \end{aligned}$$

where our convention is $|g\rangle \equiv |0\rangle$ and $|e\rangle \equiv |1\rangle$. For a logical qubit, operators are typically the products of a string of physical spin operators.

A quantum harmonic oscillator (QHO) is defined by energy eigenstates

$$\left\{ |n\rangle : E_n = \left(n + \frac{1}{2}\right) \hbar\omega_c, n = 0, 1, 2, \dots \right\}$$

and a pair of ladder operators a, a^\dagger that satisfy

$$\begin{aligned} a |n\rangle &= \sqrt{n} |n-1\rangle, \quad a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \\ [a, a^\dagger] &\equiv aa^\dagger - a^\dagger a = 1 \end{aligned}$$

A transmon qubit is a QHO with a small anharmonicity

$$\hat{H}_{tr} = 4E_C \hat{n}^2 - E_J \cos \hat{\varphi} \approx 4E_C \hat{n}^2 + \frac{1}{2} E_J \hat{\varphi}^2$$

where $E_C = \frac{e^2}{2C}$ and $E_J = \frac{\hbar^2}{4e^2 L}$

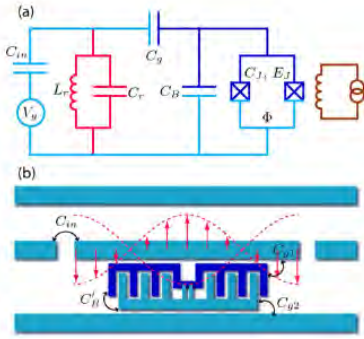


Figure 26: As the result of large $\frac{E_J}{E_C}$, the qubit is insensitive to charge fluctuation

1.2 A Variety of States

A generic pure state of a qubit is

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$\alpha, \beta \in \mathbb{C}$, normalized by

$$\langle\psi|\psi\rangle = |\alpha|^2 + |\beta|^2 = 1$$

A pure single-qubit state can be represented by a point on the Bloch sphere:

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

The state is an eigenvector of the operator $\hat{n} \cdot \vec{\sigma}$, where $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ points to the representative point on the Bloch sphere.

Density matrices in the form of $\rho = \sum_i P_i |\psi_i\rangle \langle\psi_i|$ (with $\sum_i P_i = 1$) can describe both pure and mixed states.

The key properties of density matrices are:

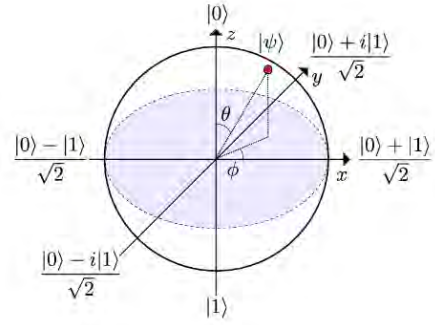


Figure 27: the Bloch sphere

- 1) Density matrices are Hermitian $\rho_{ij} = \bar{\rho}_{ji}$
- 2) The trace of a density matrix is 1 $\text{Tr}(\rho) = 1$
- 3) The eigenvalues of the density matrix are all positive and lie between 0 and 1.

For a pure state

$$\rho^2 = \rho, \quad \text{Tr}(\rho^2) = 1$$

For a mixed state (or a subsystem of an entangled state)

$$\rho^2 \neq \rho, \quad \text{Tr}(\rho^2) < 1$$

In a combined system ($\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$), a quantum state can be separable, i.e. $|\Psi\rangle = |\phi\rangle_A \otimes |\psi\rangle_B$. Its reduced density matrix (约化密度矩阵), say $\rho_A = \text{Tr}_B(\rho)$, satisfies

$$\rho_A^2 = \rho_A, \quad \text{Tr} \rho_A^2 = 1$$

More interestingly, a state can be entangled, i.e., $\text{Tr} \rho_A^2 < 1$. It encodes nontrivial mutual information, measurable by entanglement entropy(纠缠熵)

$$S_A \equiv -\text{Tr}_A(\rho_A \log_2 \rho_A) > 0$$

The well-known maximally entangled states are the Bell states, which can be distinguished and stabilized by $X_1 X_2$ and $Z_1 Z_2$.

It's not possible to perfectly clone an unknown quantum state, or a state drawn from a set of tow (or more) non-orthogonal states (quantum no-cloning theorem)(反证此定理). In other words, it's impossible to unitary evolve

$$|\psi\rangle |0\rangle \rightarrow |\psi\rangle |\psi\rangle$$

for an unknown $|\psi\rangle$ even with any environment.

Table 2: Bell states

Bell States	$X_1 X_2$	$Z_1 Z_2$
$ \Psi_{00}\rangle = \frac{ 00\rangle + 11\rangle}{\sqrt{2}}$	+1	+1
$ \Psi_{01}\rangle = \frac{ 01\rangle + 10\rangle}{\sqrt{2}}$	+1	-1
$ \Psi_{10}\rangle = \frac{ 00\rangle - 11\rangle}{\sqrt{2}}$	-1	+1
$ \Psi_{11}\rangle = \frac{ 01\rangle - 10\rangle}{\sqrt{2}}$	-1	-1

Meanwhile, the following evolution is frequently used in quantum computation and quantum communication. (纠缠)

$$(\alpha|0\rangle + \beta|1\rangle)|0\rangle \xrightarrow{CNOT} \alpha|00\rangle + \beta|11\rangle$$

1.3 Gates: Controlling the State of Qubits

Given the state of a system $|\psi(0)\rangle$ at time $t = 0$, the state of the system at time t can be expressed as

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

where $U(t)$ is called the time-evolution operator.

For time-independent Hamiltonian H , we have symbolically

$$U(t) = e^{-iHt/\hbar}$$

which leads to Schroedinger's equation

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

Such a unitary evolution is reversible operation(演化可逆).

For universal quantum computation(完备门集), we only need a small set of single-qubit gates and a two-qubit gate.

A practical scheme to control and entangle superconducting qubits is to couple them to microwave resonators, whose single EM-field mode is a QHO. This research field is known as circuit QED.

To simplify, the coupled system can often be thought of as two qubits interacting with

$$H_{int} = J_x \sigma_x^{(1)} \sigma_x^{(2)} + J_y \sigma_y^{(1)} \sigma_y^{(2)} + J_z \sigma_z^{(1)} \sigma_z^{(2)}$$

Understanding the time evolution under H_{int} is important to the design of a two-qubit quantum gate.

1.4 Entangled with Measuring Apparatuses

If $|\psi\rangle$ is the state-vector of a quantum system, and the observable L is measured, the probability to observe the eigenvalue λ is

$$P_\lambda = \langle \psi | \lambda \rangle \langle \lambda | \psi \rangle$$

where $|\lambda\rangle$ is the corresponding eigenvector. (算符代表潜在的值, 态是测出来的几率)

The state of the system immediately after the measurement is

$$\frac{|\lambda\rangle \langle \lambda | \psi \rangle}{\sqrt{P_\lambda}}$$

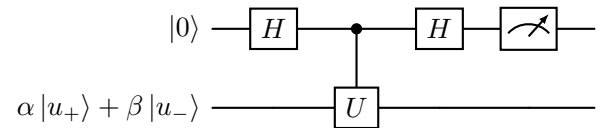
State and measurement in the quantum world are two different things. Non-orthogonal (non-identical, hence different) states cannot be reliably distinguished. (测量与态并不是一回事)

In the statistical sense, the experimental average is identical to the expectation value of M of the system (测量均值)

$$\langle M \rangle \equiv \langle \psi | M | \psi \rangle, \text{ or } \text{Tr} \rho M$$

The uncertainty of the measurement is understood as the standard deviation $\Delta M = \sqrt{\langle M^2 \rangle - \langle M \rangle^2}$ of the results measured from a large number of quantum systems in identical states.

The quantum circuit model for a measurement of an operator U acting on a single qubit is



Here, we suppose U has eigenvalues ± 1 and corresponding eigenvector $|u_\pm\rangle$. The data qubit and the measurement qubit are generically entangled in the state $\alpha|0\rangle|u_+\rangle + \beta|1\rangle|u_-\rangle$ before the projective measurement.

1.5 Decoherence: The Environment Issues

To study the combined evolution of system (S) and its environment (E), we start from a separable density matrix

$$\rho = \rho_s(0) \otimes \rho_E(0)$$

In particular, we can write

$$\rho_E(0) = |0\rangle\langle 0|$$

where $|0\rangle$ belongs to a set of environment orthogonal basis states $|i\rangle$.

Given a unitary time evolution operator $U(t)$ for the total system, the evolution of the reduced density matrix is captured by the Kraus operators $E_i = \langle i|U(t)|0\rangle$:

$$\begin{aligned}\rho_S(t) &= \text{Tr}_E \{U(t)[\rho_S(0) \otimes |0\rangle\langle 0|]U^\dagger(t)\} \\ &= \sum_i E_i \rho_S(0) E_i^\dagger\end{aligned}$$

The effects of noise are usually separated into relaxation (qubit flip)(激发态 \rightarrow 基态) and dephasing (phase randomization)(能级的能量差变化导致相位变化). (整体都称为退相干)

The energy dissipation is described by amplitude damping with

$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \quad E_1 = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}$$

The loss of quantum information without loss of energy is described by phase damping (e.g., when a photon scatters randomly as it travels through a waveguide) with

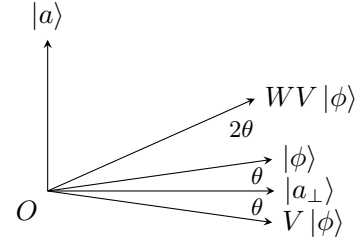
$$E_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \quad E_1 = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{p} \end{pmatrix}$$

2. The Era of NISQ Computers

They are systems that have up to thousands of qubits or even more but not full error-correction, thus noisy. They fit the term of noisy intermediate-scale quantum (NISQ) computers.

2.1 Quantum Algorithms

2.1.1 Grover's algorithm Grover's algorithm searches for an entry in an unstructured database and, thus, can be practically useful. Geometrically, the algorithm rotates a state toward the target through a series of reflections. One can show that the number of search steps goes from $O(N)$ to $O(\sqrt{N})$. If we run the algorithm once, we only have a very high probability to obtain the desired result. To ensure the success, we need to repeat the computation a few times.



We choose

$$|\phi\rangle = H^{\otimes n} |0\rangle_n = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle_n$$

Reflection V with respect to the direction of $|a_\perp\rangle$ is

$$V = 2|a_\perp\rangle\langle a_\perp| - I = I - 2|a\rangle\langle a|$$

Reflection W with respect to $|\phi\rangle$ is

$$W = 2|\phi\rangle\langle\phi| - I$$

The product of the two reflections is a rotation: WV rotates a vector through the angle 2θ . (如何计算需要转多少次)

2.2 Quantum Error Correction

(测量不相干信息进行探测纠正错误)(编码信息, 测量其是否仍在编码空间, 若不在纠正之) In the three-qubit repetition code, we measure two stabilizer generators $U_1 = Z_1 Z_2$ and $U_2 = Z_2 Z_3$.

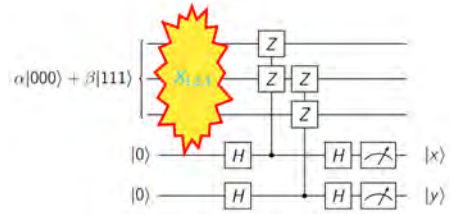


Figure 28: the three-qubit repetition code

The operators U_1 and U_2 each has two distinct eigenvalues ± 1 . The measurement of the operators, for zero and one-qubit errors, yields Therefore, the measurement

	I	X_1	X_2	X_3
$U_1 = Z_1 Z_2$	+1	-1	-1	+1
$U_2 = Z_2 Z_3$	+1	+1	-1	-1

results allows us to correct a single bit-flip error.

Surface code(容错量子计算)is a possible fault-tolerant encoding scheme. Errors can be detected by the change of measurement results. Sufficiently rare errors can be left uncorrected and undone in classical control software.

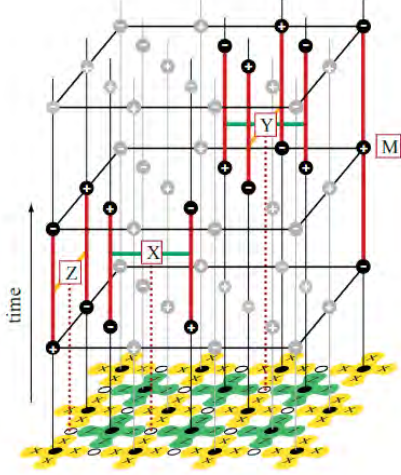


Figure 29: Surface code

3. Calculation

3.1 Tensor product

$$\mathcal{H} \rightarrow \mathcal{H}^1 \otimes \mathcal{H}^2$$

$$|0\rangle, |1\rangle \rightarrow |00\rangle, |01\rangle, |10\rangle, |11\rangle$$

$$H = \sum \vec{\sigma}_1 \vec{\sigma}_2 = \sum (\sigma_1^x \sigma_2^x + \sigma_1^y \sigma_2^y + \sigma_1^z \sigma_2^z)$$

只会有 2×2 的矩阵分解

$$H = aI + b\sigma_x + c\sigma_y + d\sigma_z$$

$$= \begin{pmatrix} d & b - ic \\ b + ic & a \end{pmatrix}$$

$$= B\hat{n}\vec{\sigma}$$

$$E_{\pm} = a \pm \sqrt{b^2 + c^2 + d^2}$$

Table 3: $\sigma \rightarrow H$

00 01 10 11

3.2 partial trace

$$|\psi\rangle = \frac{1}{\sqrt{1}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

$$\rho = |\psi\rangle\langle\psi|$$

$$\rho_A = \text{Tr}_B \rho = {}_B \langle 0|\rho|0\rangle_B + {}_B \langle 1|\rho|1\rangle_B$$

$$= \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$$

$$\langle k|U|0\rangle \rightarrow E_k$$

3.3 e^{-iHt}

$$H =$$

$$e^{-iHt} = \sum_i \frac{(-it)^j H^j}{j!}$$

3.4 Qubit Gate

单比特门 2×2

$$|\psi_{out}\rangle = U|\psi_{in}\rangle$$

双比特门 4×4

$$|\psi_{out}^{(2)}\rangle = U|\psi_{in}^{(2)}\rangle$$

3.4.1 Ctrl-Z

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix}$$

3.4.2 Swap

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$

3.4.3 $\sqrt{i}\text{Swap}$

$$\begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}$$