PHYS-C0252 - Quantum Mechanics 2021

Lecture notes

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1.1 Intended learning outcomes

- Identify how the course is technically implemented
- Identify Hilbert space and subspace of physical states
- Operate to state vectors by linear operators

1.2 Preface

Quantum mechanics is a mathematical framework to model nature. It is said to be the most successful theory in all of physics, owing to its success in describing a wide range of phenomena, including atomic orbitals, quantum tunneling, and superconductivity.

The aim of this course is to formulate quantum mechanics based on a solid mathematical foundation. We start by introducing the basic mathematical objects required to describe physical systems. Then, we introduce the postulates of quantum mechanics, and discuss how to quantize a classical system. We also consider some example systems, including qubits and a brief discussion on quantum computing. Overall, we aim to be fairly rigorous with the mathematical details, especially in the beginning, but certain subtleties are left out in order to fit more useful tools into the course. You may encounter such advanced mathematics in the Master's courses to fill in the gaps in your knowledge. To keep you on track, we intent to tell you when we do not prove of handle something rigorously.

Enjoy!

1.3 Hilbert space and kets vectors

The fundamental mathematical structure in quantum mechanics is the Hilbert space, which is a generalization of Euclidean space that may be infinite-dimensional, and whose coordinates may be complex numbers. The elements of a Hilbert space are referred to as *ket vectors*, denoted by $|\psi\rangle$. A Hilbert space $\mathcal{H}$ is a complete inner product space, which means that it has the following properties:

1. $\mathcal{H} = \{|\psi\rangle\}$ is a vector space over the scalar field $\mathbb{C}$ (see math recap on the right)
2. For any pair of elements $|\psi\rangle, |\phi\rangle \in \mathcal{H}$, there is a scalar (inner) product $\langle\psi|\phi\rangle := (|\psi\rangle, |\phi\rangle) \in \mathbb{C}$ that satisfies
   (a) $\langle\psi|\phi\rangle = (\langle\phi|\psi\rangle)^* = \langle\phi|\psi\rangle^*$ (conjugate symmetry)
   (b) $\langle\psi|a\phi_1 + b\phi_2\rangle = \langle\psi| (a|\phi_1\rangle + b|\phi_2\rangle) = a\langle\psi|\phi_1\rangle + b\langle\psi|\phi_2\rangle$ (linearity)
   (c) $\langle\psi|\psi\rangle \geq 0$; $\langle\psi|\psi\rangle = 0 \iff |\psi\rangle = 0$ (positive definiteness)
3. All Cauchy sequences converge into $\mathcal{H}$. That is, if $\exists\{|\psi_i\rangle\}$ s.t. $\| |\psi_n\rangle - |\psi_m\rangle \| \to 0$ for $n, m \to \infty$ then $\exists |\Psi\rangle \in \mathcal{H}$ s.t. $|\psi_m\rangle \to |\Psi\rangle$ for $m \to \infty$.[1]

Consequently, we can define a norm $\| |\psi\rangle \| = \|\psi\| := \sqrt{\langle\psi|\psi\rangle} \geq 0$. For example, the following inequalities apply:

- $| \langle\psi|\phi\rangle | \leq \|\psi\|\|\phi\|$, i.e., Cauchy–Schwarz inequality
- $\| |\psi\rangle + |\phi\rangle \| \leq \|\psi\| + \|\phi\|$, i.e., triangle inequality

Physical states, i.e., objects that can be used to model the states of physical systems on the quantum-mechanical level, are those elements of $\mathcal{H}$ which have a norm of unity, i.e., $\langle\psi|\psi\rangle = 1$. In this course, we use the terms *ket vector* and *state* somewhat interchangeably, since we are concerned mostly with physical states. But many of the results also hold for ket vectors with any finite norm.

Math recap on vector spaces

A vector space V over a scalar field F is a set where addition, denoted by +, is defined such that for $u, v, w \in V$, $+ : V \times V \to V$, $a, b \in F$, the following properties hold:

1. $u + (v + w) = (u + v) + w$
2. $u + v = v + u$
3. $\exists 0 \in V$ s.t. $V + 0 = V$
4. $\forall v \in V \; \exists -v \in V$ s.t. $v + (-v) = 0$
5. $a(bv) = (ab)v$
6. $1v = v$, when $1 \in F$
7. $a(u + v) = au + av$
8. $(a + b)v = av + bv$

For our purposes, the scalar field F is always either $\mathbb{R}$ or $\mathbb{C}$.

1: Not going to ask about Cauchy sequences in the exam, but this condition is what makes a Hilbert space *complete*. Thus, if you are unfamiliar with the term Cauchy sequence, no need to study it for this course.

1.4 Bra vectors

As discussed above, the ket vectors are the elements of $\mathcal{H}$, i.e., $\mathcal{H} = \{|\psi\rangle\}$. For each given ket vector $|\phi\rangle$ we symbolically define an object $\langle\phi|$, through the inner product such that for all $|\psi\rangle \in \mathcal{H}$, we have $\langle\phi|\psi\rangle := (|\phi\rangle, |\psi\rangle) \in \mathbb{C}$. Below, we justify why $\langle\phi|$ can be referred to as a bra vector, i.e., the set of all bra vectors $\{\langle\phi|\}$ forms a vector space.

For a fixed $|\phi\rangle$, the inner product $(|\phi\rangle, |\psi\rangle)$ can be identified as a mapping that takes any ket vector $|\psi\rangle$ to a complex number. Thus $\langle\phi|$ is a linear and bounded functional[2] acting on $\mathcal{H}$. The so-called Riesz representation theorem[3] states that for any linear

2: A functional f acting on a vector space V is a mapping $f : V \to \mathbb{C}$. f is said to be bounded, if $\forall v \in V$, there exists a constant M such that $|f(v)| \leq M\|v\|$.

3: Not going to ask about this in the exam.

bounded functional $\langle\phi|$, there exists a corresponding unique ket vector $|\phi\rangle \in \mathcal{H}$ such that $\langle\phi|\psi\rangle = (|\phi\rangle, |\psi\rangle)$ for all $|\psi\rangle \in \mathcal{H}$. This is the definition of the bra vector $\langle\phi|$; it is the functional whose action on any $|\psi\rangle$ corresponds to taking the inner product with the ket $|\phi\rangle$.

From the above-noted uniqueness of the ket vector $|\phi\rangle$ corresponding to its bra $\langle\phi|$, it folows that there is a one-to-one correspondence between $\mathcal{H} = \{|\psi\rangle\}$ and the set of all bra vectors $\mathcal{H}^* := \{\langle\phi|\}$. The set $\mathcal{H}^*$ is referred to as the dual space of $\mathcal{H}$.

1.5 Linear operators

Definition 1.5.1 *A mapping $\hat{A}$ is a linear operator on $\mathcal{H}$ $\Longleftrightarrow$ $\hat{A} : \mathcal{H} \to \mathcal{H}$ s.t. $\forall\, |\psi\rangle, |\phi\rangle \in \mathcal{H}$, $a, b \in \mathbb{C}$:*

$$\hat{A}\left(a\,|\psi\rangle + b\,|\phi\rangle\right) = a\hat{A}\,|\psi\rangle + b\hat{A}\,|\phi\rangle\,. \tag{1.1}$$

We denote the set of linear operators on $\mathcal{H}$ by $\mathcal{L}(\mathcal{H})$. We also define the notation

$$|\hat{A}\psi\rangle := \hat{A}\,|\psi\rangle := \hat{A}\left(|\psi\rangle\right). \tag{1.2}$$

It follows that $\forall \hat{A}, \hat{B} \in \mathcal{L}(\mathcal{H})$, we have

$$\hat{A}\left(\hat{B}\,|\psi\rangle\right) = \left(\hat{A}\hat{B}\right)|\psi\rangle\,. \tag{1.3}$$

1.6 Outer product

An important example of a linear operator is the outer product of two vectors.

Definition 1.6.1 *We define the outer product $|\psi\rangle\langle\phi| : \mathcal{H} \to \mathcal{H}$, where $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ s.t. $\forall\, |\chi\rangle \in \mathcal{H}$ we have:*

$$\left(|\psi\rangle\langle\phi|\right)|\chi\rangle = |\psi\rangle\langle\phi|\chi\rangle = \langle\phi|\chi\rangle|\psi\rangle \tag{1.4}$$

Note that in the second equality above, we moved the term $\langle\phi|\chi\rangle$ to the front, since it is simply a scalar.

Lecture 2 | 2

2.1 Intended learning outcomes

- Use bases to represent operators
- Identify the minimal mathematical structure to describe a physical system quantum mechanically

2.2 Bases of $\mathcal{H}$

Above, we have discussed bra and ket vectors in a very abstract way, without a way to visualize these vectors. To make them more tangible, we will introduce them coordinates using a basis.

Definition 2.2.1 *A set of ket vectors* $\{|\phi_i\rangle\}_{i=1}^N \in \mathcal{H}$, $N \in \mathbb{Z}_+$, *is referred to as linearly independent if* $\sum_{i=1}^N c_i |\phi_i\rangle = 0$ *implies* $c_i = 0\,\forall c_i \in \mathbb{C}$.

The *dimension* of $\mathcal{H}$, $\mathrm{Dim}\{\mathcal{H}\}$, is the largest N for which such a linearly independent set of vectors exists.

The set $\{|\phi_i\rangle\}_{i=1}^N$ is referred to as *complete* if $\forall\,|\psi\rangle \in \mathcal{H}, \exists\,\{c_k\}_{k=1}^N$, $c_k \in \mathbb{C}$ s.t. $|\psi\rangle = \sum_{k=1}^N c_k |\phi_k\rangle$.[1] That is, any ket vector in $\mathcal{H}$ may be expressed as a linear combination of the vectors $|\phi_k\rangle$. The coefficients c_k are the *coordinates* of $|\psi\rangle$. We have thus arrived at the definition of a basis:

1: Defined similarly for infinite-dimensional spaces.

Definition 2.2.2 *A complete set of linearly independent vectors* $\{|\phi_k\rangle\}$ *is referred to as a* basis *for* $\mathcal{H}$.

A basis $\{|\phi_k\rangle\}$ is referred to as *orthonormal* if

$$\langle\phi_l|\phi_m\rangle = \delta_{lm} = \begin{cases} 0, & \text{for } l \neq m, \\ 1, & \text{for } l = m. \end{cases} \tag{2.1}$$

The symbol δ_{lm} is referred to as the Kronecker delta.

An observation for the orthonormal basis $\{|\phi_k\rangle\}$: for an arbitrary $|\psi\rangle \in \mathcal{H}$, we have

$$|\psi\rangle = \sum_k c_k |\phi_k\rangle \tag{2.2}$$

$$\implies \langle\phi_m|\psi\rangle = \sum_k c_k \langle\phi_m|\phi_k\rangle = c_m. \tag{2.3}$$

Thus,

$$\begin{aligned}
|\psi\rangle &= \sum_m c_m\,|\phi_m\rangle \\
&= \sum_m \langle\phi_m|\psi\rangle|\phi_m\rangle \\
&= \sum_m |\phi_m\rangle\langle\phi_m|\psi\rangle \\
&= \left(\sum_m |\phi_m\rangle\langle\phi_m|\right)|\psi\rangle\,,
\end{aligned}$$

where in the last step, we have used the fact that the outer product is linear. Based on this, we conclude that $\sum_m |\phi_m\rangle\langle\phi_m| = \hat{I}$, the identity operator. This holds for any orthonormal basis. It is a useful trick to insert the identity operator in strategic places, and expand it in terms of an orthonormal basis like this.

2.3 States vs. vectors

For a given basis $\{|\phi_k\rangle\}$ and a ket vector $|\psi\rangle \in \mathcal{H}$, we may write

$$\begin{aligned}
|\psi\rangle &= \sum_k c_k\,|\phi_k\rangle \qquad (2.4)\\
&\triangleq \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix},
\end{aligned}$$

where $\triangleq$ stands for *represented by*. Consequently, a basis ket vector $|\phi_m\rangle$ is represented by a column vector where $c_m = 1$ and $c_k = 0$ for $k \neq m$. Note that the vector representation of a state may be infinite-dimensional.

Given a column vector representation of $|\psi\rangle$ with the coefficients $\{c_k\}$, the corresponding bra vector $\langle\psi|$ may be represented by the conjugate transpose of the column vector representing $|\psi\rangle$:

$$\langle\psi| \triangleq \begin{bmatrix} c_1^* & c_2^* & c_3^* & \dots \end{bmatrix}. \qquad (2.5)$$

This can be shown using the inner product.

2.4 Operators vs. matrices

Analogously to representing kets as column vectors, it is possible to represent operators as matrices. Let $\hat{A} \in \mathcal{L}(\mathcal{H})$ and $\{|\phi_m\rangle\}$ be an orthonormal basis of $\mathcal{H}$. Then,

$$
\begin{aligned}
\hat{A} = \hat{I}\hat{A}\hat{I} &= \left(\sum_m |\phi_m\rangle\langle\phi_m|\right) \hat{A} \left(\sum_k |\phi_k\rangle\langle\phi_k|\right) \\
&= \sum_{m,k} |\phi_m\rangle \underbrace{\langle\phi_m|\hat{A}|\phi_k\rangle}_{:=A_{mk}\in\mathbb{C}} \langle\phi_k| \\
&= \sum_{m,k} A_{mk} |\phi_m\rangle\langle\phi_k| \\
&\mathrel{\hat{=}} \begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}.
\end{aligned}
\tag{2.6}
$$

This is the *matrix representation* of the operator $\hat{A}$. Note that the matrix might be infinite-dimensional.

Using the matrix representation, the operation of $\hat{A}$ on a ket vector $|\psi\rangle$ may be written explicitly:

$$
\begin{aligned}
\hat{A}|\psi\rangle &= \sum_{m,k,l} A_{mk} |\phi_m\rangle\langle\phi_k|\phi_l\rangle \\
&= \sum_{m,k} A_{mk} c_k |\phi_m\rangle .
\end{aligned}
\tag{2.7}
$$

We observe that the expression $\sum_{m,k} A_{mk} c_k$ corresponds to matrix-vector multiplication, and conclude that

$$
\hat{A}|\psi\rangle \mathrel{\hat{=}} \begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix}.
$$

In other words, we obtain the column vector representation of $|\psi'\rangle = \hat{A}|\psi\rangle$ by calculating the matrix-vector product between the matrix representation of $\hat{A}$ and the column vector representation of $|\psi\rangle$.

Math on complex conjugation

$\forall z \in \mathbb{C}$ we have $x, y \in \mathbb{R}$ and i is the imaginary unit, then:

$$
\begin{aligned}
z &= x + iy \\
z^* &= x - iy
\end{aligned}
$$

2.5 Adjugate

Let $\hat{A} \in \mathcal{L}(\mathcal{H})$, and furthermore, let $\hat{A}$ be bounded.[2] We define the action of $\hat{A}$ on a left-lying bra vector (i.e. an element in the dual space $\mathcal{H}^*$), $\hat{A} : \mathcal{H}^* \to \mathcal{H}^*, \forall |\phi\rangle, |\psi\rangle \in \mathcal{H}$ through the relation

$$
\left(\langle\phi|\hat{A}\right)|\psi\rangle = \langle\phi|\left(\hat{A}|\psi\rangle\right). \tag{2.8}
$$

We observe that the operation $\langle\phi|\hat{A}$ is a linear functional on $\mathcal{H}$ and is bounded since $\hat{A}$ is bounded.

2: An operator $\hat{A}$ is said to be bounded if $\forall |\psi\rangle \in \mathcal{H}$ there exists a constant M such that $\|\hat{A}|\psi\rangle\| \leq M\| |\psi\rangle \|$.

About notation

These are equivalent:

$$
\begin{aligned}
\langle\phi|\hat{A}|\psi\rangle &= (|\phi\rangle, \hat{A}|\psi\rangle)) \\
&= \left(\hat{A}^\dagger|\phi\rangle, |\psi\rangle\right) \\
&= \langle\hat{A}^\dagger\phi|\psi\rangle
\end{aligned}
$$

Thus it follows from the Riesz representation theorem that $\exists\,|\phi'\rangle \in \mathcal{H}$ s.t. $\langle\phi'| = \langle\phi|\hat{A}$. This also defines a linear operator $\hat{A}^\dagger$ as

$$\hat{A}^\dagger\,|\phi\rangle = |\phi'\rangle\,, \tag{2.9}$$

which is referred to as the adjugate of $\hat{A}$.

For example, we have for $c \in \mathbb{C}$

$$\begin{aligned}\langle\phi|c|\psi\rangle &= (|\phi\rangle\,, c\,|\psi\rangle) \\ &= c\,(|\phi\rangle\,, |\psi\rangle) \\ &= (c^*\,|\phi\rangle\,, |\psi\rangle)\,,\end{aligned} \tag{2.10}$$

Thus, $c^\dagger = c^* \in \mathbb{C}$, i.e., the adjugate of a complex number is just the complex conjugate.

2.6 Properties of adjugate

The following equalities are not proven here, but proofs can be constructed based on the above definitions.

$$\left(\hat{A}^\dagger\right)^\dagger = \hat{A} \tag{2.11}$$

$$\left(a\hat{A}^\dagger\right)^\dagger = a^*\hat{A} \qquad (a \in \mathbb{C}) \tag{2.12}$$

$$\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger \tag{2.13}$$

$$\left(|\psi\rangle\langle\phi|\right)^\dagger = |\phi\rangle\langle\psi| \tag{2.14}$$

Furthermore, given a matrix representation A of $\hat{A}$, the matrix representation of $\hat{A}^\dagger$ is given by the conjugate transpose of A, which is obtained by taking the transpose and then the complex conjugate of each element of A.

2.7 Eigenvalues and eigenstates

For an operator $\hat{A} \in \mathcal{L}(\mathcal{H})$, if a ket vector $|\psi_k\rangle \in \mathcal{H}$ satisfies the *eigenvalue equation*

$$\hat{A}\,|\psi_k\rangle = \lambda_k\,|\psi_k\rangle \tag{2.15}$$

for some scalar $\lambda_k \in \mathbb{C}$, we define $|\psi_k\rangle$ to be an eigenvector, or eigenstate, of $\hat{A}$ with an eigenvalue λ_k. The subscript k signifies that there may be (infinitely) many eigenstates and corresponding eigenvalues.

The set of eigenvalues $\{\lambda_k\}$ is referred to as the *spectrum* of $\hat{A}$.

It is possible that for a given eigenvalue λ_k, there are multiple eigenvectors $|\psi_{k,i}\rangle$ that satisfy Eq. (2.15), with $i = 1, \dots, g_k$. The number of eigenvectors g_k corresponding to λ_k is referred to as the *degeneracy* of λ_k.

2.8 Hermitian operators

Definition 2.8.1 *The operator $\hat{H} \in \mathcal{L}(\mathcal{H})$ is defined to be Hermitian iff*[3] $\hat{H}^\dagger = \hat{H}$.

3: If and only if

Hermitian operators are very important in quantum mechanics as discovered below.

The key feature of Hermitian operators comes from the so-called generalized spectral theorem, which states that for a Hermitian operator $\hat{H} \in \mathcal{L}(\mathcal{H})$, there exists a complete orthonormal basis of $\mathcal{H}$, $\{|\psi_k\rangle\}$, which satisfies

$$\hat{H} |\psi_k\rangle = \lambda_k |\psi_k\rangle . \tag{2.16}$$

Importantly, it also follows from the spectral theorem that the eigenvalues λ_k are real numbers.

The above result implies that for any Hermitian operator $\hat{H}$, it is always possible to find a basis such that

$$\hat{H} = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k| . \tag{2.17}$$

In the matrix representation, this is a matrix with just the eigenvalues λ_k on the diagonal. This is useful for many reasons. For one, it is very easy to operate on any vector with such an operator. Furthermore, it turns out that many problems in quantum mechanics boil down to finding the eigenvalues of Hermitian operators. The process of finding such a basis in which the eigenvalues are on the diagonal is referred to as *diagonalization*, and much of the effort in theoretical physics is spent on trying to diagonalize operators related to different physical systems.

2.9 Postulates of quantum mechanics

We finally have introduced all the necessary mathematics to start discussing physical systems. The theory of quantum mechanics is in essence built upon the six *postulates* discussed below. They are the fundamental assumptions, or axioms, of quantum mechanics, i.e., they are not proven, but rather they are based on empirical evidence. Predictions derived from the postulates have been experimentally verified to extremely high precision. In this course, we consider quantum mechanics simply as a model for such experimental observations.

Postulate I

For each physical system there exists a corresponding (rigged)[4] Hilbert space.

4: We discuss this later

Postulate II

Each physical state of this system can be represented by a quantum state $|\psi\rangle \in \mathcal{H}$, where $\langle\psi|\psi\rangle = 1$.

Postulate III

For each measurable quantity A of the system we have a corresponding operator $\hat{A} \in \mathcal{L}(\mathcal{H})$ s.t. $\hat{A}^\dagger = \hat{A}$. Such an operator (and often also the corresponding quantity) is referred to as an *observable* of the system.

In an ideal measurement of the quantity A, any measurement outcome equals to an eigenvalue of $\hat{A}$.[5]

5: Recall that since $\hat{A}$ is Hermitian, this implies that all measurement outcomes are real numbers, as one would expect.

Postulate IV: Measurement

Let $|\psi\rangle \in \mathcal{H}$ and $\hat{A}^\dagger = \hat{A} \in \mathcal{L}(\mathcal{H})$ with a discrete spectrum $\{a_n\}$. As discussed in Sec. 2.8, there always exists an orthonormal basis for $\mathcal{H}$, $\{|\phi_{n,i}\rangle\}_{n,i=\in\{1,\ldots,g_n\}}$, where g_n is the amount of degeneracy, such that the basis vectors are eigenstates of $\hat{A}$.

The probability of obtaining a specific measurement result a_n is given by

$$P(a_n) \coloneqq \sum_{i=1}^{g_n} \left|\langle\phi_{n,i}|\psi\rangle\right|^2 . \tag{2.18}$$

Postulate V: Effect of measurement on the state

Suppose that a system is in the state $|\psi\rangle \in \mathcal{H}$. If we measure the quantity corresponding to $\hat{A}$ and obtain the measurement result

a_n (an eigenvalue of $\hat{A}$), the state of the system *collapses* into the state

$$|\psi'\rangle = \frac{\hat{P}_n |\psi\rangle}{\|\hat{P}_n |\psi\rangle\|}, \qquad \hat{P}_n = \sum_{i=1}^{g_n} |\phi_{n,i}\rangle\langle\phi_{n,i}| \,. \tag{2.19}$$

$\hat{P}_n$ is referred to as a projector onto the subspace corresponding to the subspace spanned by the eigenstates $\{|\phi_{n,i}\rangle\}_{i=1}^{g_n}$.

Definition 2.9.1 *$\hat{P}_n \in \mathcal{L}(\mathcal{H})$ is a projector iff $\hat{P}_n^2 = \hat{P}_n$.*

Postulate VI: Temporal evolution

If a system is in the state $|\psi\rangle$, the temporal evolution of the state $|\psi(t)\rangle$ is determined by the *Schrödinger equation*:

$$\mathrm{i}\hbar\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \,, \tag{2.20}$$

where $\partial_t := \frac{\partial}{\partial t}$, $\hbar = 1.0545718 \times 10^{-34}$ Js is the reduced Planck constant, and $\hat{H} = \hat{H}^\dagger$, $\hat{H} \in \mathcal{L}(\mathcal{H})$ is the *Hamiltonian*, the observable corresponding to the total energy of the system.[6]

6: The measurable quantity corresponding to the observable $\hat{H}$ is the Hamiltonian H from classical Hamiltonian mechanics.

Note that $\hat{H}$ may also depend on time through temporally dependent parameters $\{\alpha_i(t)\}$, i.e., $\hat{H} = \hat{H}\,[\alpha_1(t), \alpha_2(t), \ldots]$. This is discussed later.

Lecture 3 | 3

3.1 Intended learning outcomes

- Differentiate between a measurement outcome and its expectation value
- Identify continuous bases for Hilbert spaces
- Apply Lagrangian formalism to quantize physical systems

3.2 Expectation values

Definition 3.2.1 *Let $\hat{A} \in \mathcal{L}(\mathcal{H})$ and $|\psi\rangle \in \mathcal{H}$. The expectation value of $\hat{A}$ when the system is in the state $|\psi\rangle$ is defined by*

$$\langle A \rangle := \langle \psi | \hat{A} | \psi \rangle \,. \tag{3.1}$$

In particular, if we have an observable quantity A with a corresponding Hermitian operator $\hat{A}$, the expectation value is equal to the classical expectation value $\langle A \rangle$ of A. That is, repeatedly preparing the system in the state $|\psi\rangle$ and measuring A, one obtains on average the result $\langle A \rangle$, even though individual measurements only yield discrete values a_k, the eigenvalues of $\hat{A}$.

Mathematically, the above discussion maybe considered as follows: Recall that $\hat{A} = \hat{A}^\dagger$ implies that there exists an orthonormal basis $\{|\phi_k\rangle\}$ such that $\hat{A}\,|\phi_k\rangle = a_k\,|\phi_k\rangle$, $a_k \in \mathbb{R}$. Subsequently, we write the state as $|\psi\rangle = \sum_k c_k\,|\phi_k\rangle$, from which we obtain

$$\begin{aligned}
\langle \psi | \hat{A} | \psi \rangle &= \left(\sum_k c_k\,|\phi_k\rangle \right)^\dagger \hat{A} \sum_k c_k\,|\phi_k\rangle \\
&= \left(\sum_k c_k\,|\phi_k\rangle \right)^\dagger \sum_k c_k a_k\,|\phi_k\rangle \\
&= \sum_{n,k} c_n^* a_k c_k\,\langle \phi_n | \phi_k \rangle \\
&= \sum_k a_k \underbrace{|c_k|^2}_{P(a_k)} = \sum_k a_k P(a_k).
\end{aligned} \tag{3.2}$$

The sum on the right side of the last equality above is the classical definition of the expectation value for the measurement outcomes.

3.3 Variance

Definition 3.3.1 *We define the variance of $\hat{A}$ when the system is in the state $|\psi\rangle$ as*

$$\begin{aligned} \Delta A^2 &= \langle\psi| \left(\hat{A} - \langle\psi|\hat{A}|\psi\rangle\right)^2 |\psi\rangle \\ &= \langle\psi|\hat{A}^2|\psi\rangle - \left(\langle\psi|\hat{A}|\psi\rangle\right)^2 \\ &= \sum_k a_k^2 P_k - \left(\sum_k a_k P_k\right)^2 . \end{aligned} \tag{3.3}$$

As above in the case of the expectation value, if $\hat{A}$ is a Hermitian operator corresponding to the observable A, the above definition coincides with that of the classical variance of A.

3.4 Continuous bases

Continuous bases are sometimes required, for example, if continuous variables are used.

Let $\{|\psi_\alpha\rangle\} \in \mathcal{H}$, where $\alpha, \alpha' \in \mathbb{R}$ s.t.

$$\langle\psi_\alpha|\psi_{\alpha'}\rangle = \delta(\alpha - \alpha'), \tag{3.4}$$

where $\delta(x)$ is the Dirac delta function. Such a set of vectors is a continuous base for $\mathcal{H}$.

Math on Dirac delta function

For a smooth function, i.e., $f \in C^\infty$:

$$\int \mathrm{d}x\{\delta(x)f(x)\} = f(0)$$

Note that $\langle\psi_\alpha|\psi_\alpha\rangle = \delta(0) = \infty$. Thus $|\psi_\alpha\rangle$ is not possible to normalize. This is why we consider *rigged* Hilbert spaces, which allow such states.[1]

1: It is possible to verify that all the properties of a Hilbert space hold even with such non-normalizable states, but it is fairly laborious and therefore we do not discuss it further.

Now, similarly as for discrete bases, we may write any $|\psi\rangle \in \mathcal{H}$ using this basis, but with an integral instead of a sum:

$$\begin{aligned} |\psi\rangle &= \int c_\alpha |\psi_\alpha\rangle \,\mathrm{d}\alpha \\ &= \int \langle\psi_\alpha|\psi\rangle|\psi_\alpha\rangle \,\mathrm{d}\alpha \\ &= \int |\psi_\alpha\rangle\langle\psi_\alpha|\psi\rangle \,\mathrm{d}\alpha = \underbrace{\left(\int |\psi_\alpha\rangle\langle\psi_\alpha| \,\mathrm{d}\alpha\right)}_{\hat{I}} |\psi\rangle \end{aligned} \tag{3.5}$$

Note that the index $\alpha \in \mathbb{R}$ of the coefficients $c_\alpha \in \mathbb{C}$ is continuous. Often, instead of c_α we write $\langle\psi_\alpha|\psi\rangle := \psi(\alpha)$, where $\psi(\alpha) : \mathbb{R} \to \mathbb{C}$ is generally referred to as the *wave function*.

Typically, the wave function is expressed in the position basis $\{|x\rangle\}$, i.e., $\psi(x) := \langle x|\psi\rangle$. From the above equation it follows that the probability density for the particle to reside at position x is given by $|\psi(x)|^2$. Note that the wave function cannot fully describe all quantum systems, just those where such continuous variables exist and are sufficient.

Definition 3.4.1 *In a continuous basis, the measurement probability of the measurement outcome to reside in* $[\alpha, \alpha + d\alpha]$ *is defined by*

$$dP(\alpha) = |\langle\psi_\alpha|\psi\rangle|^2 \, d\alpha. \tag{3.6}$$

3.5 Commutators

Definition 3.5.1 *The* commutator *of* $\hat{A}, \hat{B} \in \mathcal{L}(\mathcal{H})$ *is given by*

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

If two operators satisfy $[\hat{A}, \hat{B}] = 0$*, i.e.,* $\hat{A}\hat{B} = \hat{B}\hat{A}$*, it is defined that* $\hat{A}$ *and* $\hat{B}$ commute.

The commutator is an important operation between two operators and appears in numerous places in quantum mechanics.

3.6 Classical pendulum

Above, we introduced how to connect mathematics to physics through the postulates. The Hamiltonian of the system is the key here. Once one has it, also the relevant Hilbert space arises from its eigenstates in addition to the temporal evolution of any state. However, how do we obtain the Hamiltonian for the system?

To answer this question, we take a slight detour to classical mechanics. As an illustrative example, we discuss a classical pendulum, and construct the classical Hamiltonian for it. Subsequently, in the next section, we provide a general procedure, or recipe, for converting the classical Hamiltonian of any system to the corresponding quantum Hamiltonian. In the next lecture, we use the obtained Hamiltonian for the pendulum to describe the quantum harmonic oscillator.

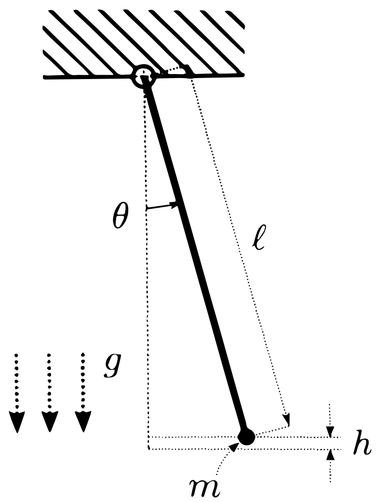

Figure 3.1: Ideal classical pendulum, where a mass m is attached to a massless rigid rod of length l. The rod may rotate without friction about a single axis as described by the angle θ. We assume a uniform gravitational field described by g.

Recall from classical mechanics that a system with N degrees of freedom can be described by a set of N generalized coordinates $\{q_i\}_{i=1}^N$. The coordinates may for example be just the position of a particle, but often the description of the system is drastically simplified if one chooses the generalized coordinates wisely.

We consider the pendulum shown in Fig. 3.1. Even though the mass at the end of the pendulum moves in a 2D plane, we recognize that there is only one degree of freedom in the system; the position is fully determined by the angle θ. We thus choose the generalized position

$$q = l\theta. \tag{3.7}$$

We drop the subscript i because we have only one degree of freedom, but all the definitions below apply in general for multidimensional systems as well.

The potential energy V depends only on q, and not on the time derivative $\dot{q}$. For small θ, it assumes the form

$$\begin{aligned} V &= gmh \\ &= mgl\,(1-\cos\theta) \approx \frac{1}{2}mgl\theta^2 = \frac{mg}{2l}q^2. \end{aligned} \tag{3.8}$$

Math on dot notation

$$\dot{y} = \frac{\mathrm{d}y}{\mathrm{d}t} \underbrace{\neq}_{\text{generally}} \frac{\partial y}{\partial t}$$

Math on Taylor series

$$\cos x = 1 - \frac{x^2}{2} + \frac{x^4}{24} - \cdots$$

It is straightfoward to write the kinetic energy T in terms of $\dot{q}$:

$$T = \frac{1}{2}mv^2 = \frac{1}{2}ml^2\dot{\theta}^2 = \frac{1}{2}m\dot{q}^2. \tag{3.9}$$

Definition 3.6.1 *The* Lagrangian *is defined as*

$$L := T - V. \tag{3.10}$$

Thus, the Lagrangian for our case is

$$\begin{aligned} L = T - V &= \frac{1}{2}ml^2\dot{\theta}^2 - \frac{1}{2}mgl\theta^2 \\ &= \frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2. \end{aligned} \tag{3.11}$$

Definition 3.6.2 *The* generalized momentum *corresponding to the coordinate q_i is defined as*

$$p_i := \frac{\partial L}{\partial \dot{q}_i}.$$

Note that when computing the momentum from the Lagrangian, q_i and $\dot{q}_i$ should be considered independent variables. Using the above definition, the generalized momentum is (again, dropping the subscript)

$$p = \frac{\partial}{\partial \dot{q}}\left(\frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2\right) = m\dot{q}. \tag{3.12}$$

Definition 3.6.3 *The classical Hamiltonian is defined as*

$$H := \sum_i \dot{q}_i p_i - L.$$

Using this, we obtain the Hamiltonian of the pendulum (i.e. the 1D harmonic oscillator):

$$\begin{aligned} H = \dot{q}p - L = m\dot{q}^2 - \left(\frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2\right) \\ = \frac{p^2}{2m} + \frac{mg}{2l}q^2 = T + V. \end{aligned} \tag{3.13}$$

3.7 Quantizing a classical system

The term *quatization* refers to the process of building a quantum-mechanical model from the classical description of the system in question. In general, given the classical Hamiltonian of a system, it can be quantized using the following procedure:

1. **Operator substitution:** Replace all generalized positions and momenta with corresponding Hermitian operators, simply by writing hats on the classical quantities:

$$\begin{aligned} q_i \longrightarrow \hat{q}_i, \quad \hat{q}_i : \mathcal{H} \to \mathcal{H}, \quad \hat{q}_i = \hat{q}_i^\dagger, \\ p_i \longrightarrow \hat{p}_i, \quad \hat{p}_i : \mathcal{H} \to \mathcal{H}, \quad \hat{p}_i = \hat{p}_i^\dagger. \end{aligned}$$

2. **Quantized Hamiltonian:** Using step 1, convert the classical Hamiltonian H to the operator $\hat{H}$, i.e., replace all classical generalized positions and momenta in H by their quantum mechanical counterparts.
3. **Canonical commutation relation:** It follows from the postulates, that the positions and momenta must satisfy $[\hat{p}_i, \hat{q}_i] = \hat{p}_i\hat{q}_i - \hat{q}_i\hat{p}_i = -i\hbar$, which is referred to as the *canonical commutation relation* (CCR).
4. **Temporal evolution:** With the above operators and the constraint imposed by the CCR, the temporal evolution of the system is given by the Schrödinger equation $i\hbar\partial_t |\psi\rangle = \hat{H} |\psi\rangle$.

For the pendulum discussed above, the quantization procedure simply yields

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mg}{2l}\hat{q}^2. \tag{3.14}$$

The significance of the CCR and the temporal evolution for the harmonic oscillator will be discussed on the following lectures.

The above procedure maybe used for many different systems. For example, it is possible to quantize electric circuits by choosing charge as the generalized position and magnetic flux as the momentum, or vice versa.[2] Another important application is the quantization of the electromagnetic field, which follows a similar procedure but with a continuous set of generalized coordinates.

2: This is discussed in the Quantum Circuits course.

Lecture 4 | 4

4.1 Intended learning outcomes

- Apply creation and annihilation operators for a harmonic oscillator
- Apply canonical commutation relations
- Identify Heisenberg's uncertainty relation

4.2 One-dimensional quantum harmonic oscillator

As we derived above in Eq. (3.14), the operator corresponding to the classical Hamiltonian of the harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\underbrace{\frac{g}{l}}_{=:\omega^2}\hat{q}^2 \tag{4.1}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{4.2}$$

where $[\hat{q}, \hat{p}] = \mathrm{i}\hbar$, $\hat{q} = \hat{q}^\dagger$, $\hat{p} = \hat{p}^\dagger$.

Next, we wish to solve the eigenstates of the oscillator. To this end, we try to rewrite the Hamiltonian in the following form, with $A, B, C \in \mathbb{R}$:

$$\hat{H} = (A\hat{q} - \mathrm{i}B\hat{p})\,(A\hat{q} + \mathrm{i}B\hat{p}) + C. \tag{4.3}$$

With some algebraic manipulation and the help of the CCR, we find

$$\begin{aligned}\hat{H} &= A^2\hat{q}^2 + \mathrm{i}AB\hat{q}\hat{p} - \mathrm{i}B\hat{p}A\hat{q} + B^2\hat{p}^2 + C \\ &= A^2\hat{q}^2 + B^2\hat{p}^2 + \underbrace{\mathrm{i}AB\underbrace{[\hat{q}, \hat{p}]}_{=\mathrm{i}\hbar}}_{=-\hbar BA} + C.\end{aligned} \tag{4.4}$$

Math on $\mathbb{C}$

For $x, y \in \mathbb{R}$,

$$(x + y)(x - y) = x^2 - y^2$$

$$\underbrace{(x + \mathrm{i}y)}_{=:z}\underbrace{(x - \mathrm{i}y)}_{=z^*} = x^2 + y^2 = |z|^2$$

Comparing this to Eq. (4.2), we choose

$$A = \sqrt{\frac{1}{2}m\omega^2}, \tag{4.5}$$

$$B = \sqrt{\frac{1}{2m}}, \tag{4.6}$$

$$C = \hbar AB = \frac{\hbar\omega}{2}. \tag{4.7}$$

With these, we may write

$$\begin{aligned}
\hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 \\
&= \left(\hat{q}\sqrt{\frac{m\omega^2}{2}} + \mathrm{i}\hat{p}\sqrt{\frac{1}{2m}}\right)^\dagger \left(\hat{q}\sqrt{\frac{m\omega^2}{2}} + \mathrm{i}\hat{p}\sqrt{\frac{1}{2m}}\right) + \frac{1}{2}\hbar\omega \\
&= \hbar\omega\left[\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right)^\dagger}_{=\hat{a}^\dagger} \underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right)}_{=:\hat{a}} + \frac{1}{2}\right] \\
&= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).
\end{aligned} \tag{4.8}$$

Definition 4.2.1 *For the one-dimensional quantum harmonic oscillator, we define*

$$\hat{a} := \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right),$$

from which is follows that

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

and

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

.

The operator $\hat{a}$ is referred to as the *lowering* or *annihilation operator* and $\hat{a}^\dagger$ is referred to as the *raising* or *creation operator*. Sometimes, $\hat{a}$ and $\hat{a}^\dagger$ together are referred to as *ladder operators*.

Note that $\hat{a} \neq \hat{a}^\dagger$, i.e. $\hat{a}$ is not Hermitian, which means that it does not correspond to an observable. However, the product $\hat{a}^\dagger\hat{a}$ is Hermitian. Thus it is enough to find its eigenvalues and eigenstates to solve the quantum-mechanical problem of the harmonic oscillator.

Let us calculate the commutator of $\hat{a}$ and $\hat{a}^\dagger$ as

$$\begin{aligned} [\hat{a}, \hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left[\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}, \hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p}\right] \\ &= \frac{m\omega}{2\hbar}\left[\hat{q}, -\frac{\mathrm{i}}{m\omega}\hat{p}\right] + \left[\frac{\mathrm{i}}{m\omega}\hat{p}, \hat{q}\right] \\ &= \frac{\mathrm{i}}{2\hbar}\big(- \underbrace{[\hat{q}, \hat{p}]}_{=\mathrm{i}\hbar} + \underbrace{[\hat{p}, \hat{q}]}_{=-\mathrm{i}\hbar} \big) = 1. \end{aligned} \tag{4.9}$$

Some observations about the quantum harmonic oscillator:

1. $\langle\psi|\hat{H}|\psi\rangle \geq 0 \;\forall\, |\psi\rangle$, since

$$\begin{aligned} \langle\hat{H}\rangle &= \langle\psi|\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|\psi\rangle \\ &= \frac{\hbar\omega}{2} + \langle\psi|\hbar\omega\hat{a}^\dagger\hat{a}|\psi\rangle \\ &= \hbar\omega\left(\frac{1}{2} + \|\hat{a}\,|\psi\rangle\,\|^2\right) \geq 0. \end{aligned} \tag{4.10}$$

   Thus all eigenenergies are positive.
2. Let $|\psi\rangle$ be an eigenstate of $\hat{H}$ s.t. $\hat{H}\,|\psi\rangle = \varepsilon\,|\psi\rangle$. Then,

$$\begin{aligned} \hat{H}\hat{a}\,|\psi\rangle &= \hbar\omega\Big(\underbrace{\hat{a}^\dagger\hat{a}}_{=\hat{a}\hat{a}^\dagger-1} + \frac{1}{2}\Big)\hat{a}\,|\psi\rangle \\ &= \hat{a}\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2} - 1\right)|\psi\rangle \\ &= \hat{a}\left(\hat{H} - \hbar\omega\right)|\psi\rangle \\ &= \hat{a}\,(\varepsilon - \hbar\omega)\,|\psi\rangle = (\varepsilon - \hbar\omega)\hat{a}\,|\psi\rangle\,. \end{aligned} \tag{4.11}$$

   In other words, $|\psi'\rangle = \hat{a}\,|\psi\rangle$ is also an eigenstate of $\hat{H}$, with energy $\varepsilon - \hbar\omega$. Similarly, we have $\hat{H}\hat{a}^\dagger\,|\psi\rangle = (\varepsilon + \hbar\omega)a^\dagger\,|\psi\rangle$. Thus, $\hat{a}$ lowers and $\hat{a}^\dagger$ raises the energy of the state $|\psi\rangle$ by one quantum of energy $\hbar\omega$. This is where their names come from.

From points 1. and 2., it follows that there exists a state $|0\rangle \in \mathcal{H}$ s.t. $\hat{a}\,|0\rangle = 0$. Thus, $|0\rangle$ is referred to as the *ground state*, i.e., the state with the lowest possible energy. Let us find the energy of the oscillator in the state $|0\rangle$:

$$\begin{aligned} \hat{H}\,|0\rangle &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|0\rangle \\ &= \frac{\hbar\omega}{2}\,|0\rangle\,. \end{aligned} \tag{4.12}$$

Thus the spectrum of $\hat{H}$ is $\{\varepsilon_n\} = \left\{\hbar\omega\left(n + \frac{1}{2}\right)\right\}$, and the corresponding eigenstates are simply written as $\{|n\rangle\}$. That is, $\hat{H}\,|n\rangle =$

$\hbar\omega\left(n+\frac{1}{2}\right)|n\rangle$.

4.3 Symbolic operator differential

Let $\hat{q}$ and $\hat{p}$ be a conjugate pair and $\hat{q}$ be such that it has a continuous spectrum.

Such a conjugate pair satisfies the commutation relation $[\hat{q},\hat{p}]=\mathrm{i}\hbar$. Some calculations are simplified if we symbolically define $\hat{p}=-\mathrm{i}\hbar\partial_{\hat{q}}$, where $\partial_{\hat{q}}$ means we take symbolically the derivative w.r.t. $\hat{q}$. We will check below that this symbolical differentiation is consistent with the commutation relation.

For example, $\forall\,|\psi\rangle\in\mathcal{H}$

$$\partial_{\hat{q}}f(\hat{q})\,|\psi\rangle=\left(f'(\hat{q})+f(\hat{q})\partial_{\hat{q}}\right)|\psi\rangle\,, \tag{4.13}$$

where f is a continuously differentiable function and f' denotes its derivative.

Let us check the above claim that $[\hat{q},\hat{p}]=\mathrm{i}\hbar$ when $\hat{p}=-\mathrm{i}\hbar\partial_{\hat{q}}$:

$$\begin{aligned}[\hat{q},\hat{p}] &= \hat{q}\hat{p}-\hat{p}\hat{q} \qquad (4.14)\\ &= \hat{q}\left(-\mathrm{i}\hbar\partial_{\hat{q}}\right)-\left(-\mathrm{i}\hbar\partial_{\hat{q}}\right)\hat{q}\\ &= -\mathrm{i}\hbar\hat{q}\partial_{\hat{q}}+\mathrm{i}\hbar\partial_{\hat{q}}\hat{q}\\ &= -\mathrm{i}\hbar\hat{q}\partial_{\hat{q}}+\mathrm{i}\hbar\underbrace{\left(\partial_{\hat{q}}\hat{q}\right)}_{=\hat{I}}+\mathrm{i}\hbar\hat{q}\partial_{\hat{q}}\\ &= \mathrm{i}\hbar.\end{aligned}$$

4.4 Solving the ground state in the position representation

Using the fact that $\hat{a}\,|0\rangle=0$ and the above definition of the symbolic differential, we have

$$\begin{aligned}0 &= \langle x'|\hat{a}|0\rangle \qquad (4.15)\\ &= \langle x'|\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x}+\frac{\mathrm{i}}{m\omega}(-\mathrm{i}\hbar\partial_{\hat{x}})\right)}_{=\hat{a}}\underbrace{\left(\int \mathrm{d}\tilde{x}\,|\tilde{x}\rangle\langle\tilde{x}|\right)}_{=\hat{I}}|0\rangle\\ &= \sqrt{\frac{m\omega}{2\hbar}}\int \mathrm{d}\tilde{x}\,\underbrace{\langle x'|\tilde{x}\rangle}_{\delta(\tilde{x}-x')}\left(\tilde{x}+\frac{\hbar}{m\omega}\partial_{\tilde{x}}\right)\underbrace{\psi_0(\tilde{x})}_{=:\langle\tilde{x}|0\rangle}\end{aligned}$$

$$\Rightarrow \left(x + \frac{\hbar}{m\omega}\partial_x\right)\psi_0(x) = 0 \tag{4.16}$$

$$\Rightarrow \psi_0(x) = C\exp\left(-\frac{x^2 m\omega^2}{2\hbar}\right), \tag{4.17}$$

where $C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$ is a normalization coefficient.

We may further derive the wave function of the first excited state from $\psi_1(x) = \tilde{C}\langle x|\hat{a}^\dagger|1\rangle$ where we do not even need to solve a differential equation since we know $\psi(x)_0$ and we may simply multiply it and take the first derivative. Similarly, we may proceed to derive the wave function of any state $|n\rangle$. However, we do not do this here, but come back to the harmonic oscillator on the second half of the course where we study the wave functions of the excited states further.

4.5 Uncertainty relations

Definition 4.5.1 *The Heisenberg uncertainty relation is defined as*

$$\Delta q \Delta p \geq \frac{\hbar}{2}, \tag{4.18}$$

where $\Delta A^2 = \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2$ *and* $[\hat{q},\hat{p}] = i\hbar$ *since* $\hat{q}$ *and* $\hat{p}$ *are a canonical conjugate pair*[1] .

1: *Warning:* does not strictly speaking apply if an operator is not bounded

Definition 4.5.2 *The Robertson uncertainty relation is defined as*

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right|, \tag{4.19}$$

where $\hat{A},\hat{B} \in \mathcal{L}(\mathcal{H})$ *may be unbounded,* $\hat{A} = \hat{A}^\dagger$, $\hat{B} = \hat{B}^\dagger$, *and* $\langle\cdot\rangle := \langle\psi|\cdot|\psi\rangle$.

Let us prove the above relations. To this end, we define $|f\rangle = \left(\hat{A} - \langle\hat{A}\rangle\right)|\psi\rangle$ and $|g\rangle = \left(\hat{B} - \langle\hat{B}\rangle\right)|\psi\rangle$. Then,

Math on norm of $\mathbb{C}$

For $z \in \mathbb{C}$,

$$|z|^2 = (\text{Re } z)^2 + (\text{Im } z)^2$$
$$\geq (\text{Im } z)^2 = \left(\frac{z - z^*}{2i}\right)^2$$

$$\begin{aligned}\Delta A^2 &= \langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\right)^2|\psi\rangle \\ &= \underbrace{\langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)}_{\left(\left(\hat{A}-\langle\hat{A}\rangle\hat{I}\right)|\psi\rangle\right)^\dagger}\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)|\psi\rangle \\ &= \langle f|f\rangle = \||f\rangle\|^2,\end{aligned} \tag{4.20}$$

and similarly,

$$\Delta B^2 = \langle g|g\rangle = \||g\rangle\|^2. \tag{4.21}$$

Then, the Cauchy–Schwarz inequality implies

$$
\begin{aligned}
|\langle f|g\rangle| &\leq \| |f\rangle \| \, \| |g\rangle \| && (4.22)\\
\Rightarrow \Delta A^2 \Delta B^2 &\geq |\underbrace{\langle f|g\rangle}_{\in\mathbb{C}}|^2 && (4.23)\\
&= \left|\langle\psi| \left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)\left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)|\psi\rangle\right|^2\\
&\geq \frac{\left|\langle\psi| \left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)\left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)|\psi\rangle - \langle\psi| \left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)|\psi\rangle\right|^2}{4}\\
&= \frac{\left|\langle\psi|[\hat{A} - \langle\hat{A}\rangle\hat{I}, \hat{B} - \langle\hat{B}\rangle\hat{I}]|\psi\rangle\right|^2}{4}\\
&= \frac{\left|\langle[\hat{A}, \hat{B}]\rangle\right|^2}{4} \quad \square
\end{aligned}
$$

Lecture 5 | 5

5.1 Intended learning outcomes

- Apply the operator exponential to symbolically solve the Schrödinger equation
- Differentiate between a qubit and a general quantum system
- Represent a qubit state on the Bloch sphere

5.2 Unitary temporal evolution

Let $|\psi(t)\rangle \in \mathcal{H}$ and $\hat{H} \in \mathcal{L}(\mathcal{H})$ be the Hamiltonian of a system. Let $|\psi(t=0)\rangle = |\psi(0)\rangle$ be the initial state of the system, the state at $t = 0$. As discussed before, the temporal evolution is then given by the Schrödinger equation:

$$\begin{aligned} \mathrm{i}\hbar\partial_t |\psi(t)\rangle &= \hat{H} |\psi(t)\rangle \\ \iff \partial_t |\psi(t)\rangle &= -\frac{\mathrm{i}\hat{H}}{\hbar} |\psi(t)\rangle . \end{aligned} \tag{5.1}$$

Note that we have assumed that $\hat{H}$ is independent of time.

Definition 5.2.1 *For $\hat{A} \in \mathcal{L}(\mathcal{H})$, let*

$$\mathrm{e}^{\hat{A}} := \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}. \tag{5.2}$$

Note that in general $\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} \neq \mathrm{e}^{\hat{A}+\hat{B}}$. The equality holds if $\hat{A}$ and $\hat{B}$ commute. [1]

1: The general expression for $\hat{C}$ in $\mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}} = \mathrm{e}^{\hat{C}}$ is given by the *Baker–Campbell–Hausdorff formula*.

With this definition,

$$\begin{aligned} \partial_t \mathrm{e}^{\hat{A}t} &= \partial_t \left(\sum_{n=0}^{\infty} \frac{\hat{A}^n t^n}{n!} \right) \\ &= \sum_{n=1}^{\infty} \frac{\hat{A}^n n t^{n-1}}{n!} \\ &= \hat{A} \sum_{n=1}^{\infty} \frac{(\hat{A}t)^{n-1}}{(n-1)!} \\ &= \hat{A} \sum_{n=0}^{\infty} \frac{(\hat{A}t)^{n}}{n!} \\ &= \hat{A}\mathrm{e}^{\hat{A}t}. \end{aligned} \tag{5.3}$$

Math on a diff.eq.

$$\partial_x f(x) = \lambda f(x) \implies f(x) = A\mathrm{e}^{\lambda x}$$

The temporal evolution can then be written as

$$\begin{aligned} |\psi(t)\rangle &= \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,|\psi(0)\rangle \\ &=: \hat{U}(t)\,|\psi(0)\rangle\,, \end{aligned} \tag{5.4}$$

where $\hat{U}(t) = \exp\left(-\mathrm{i}\hat{H}t/\hbar\right)$ is the *time-evolution operator*, or sometimes referred to as the *propagator* of the system.

Recalling that $\hat{H}^\dagger = \hat{H}$, we observe that

$$\begin{aligned} \hat{U}(t)^\dagger &= \left(\mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\right)^\dagger \\ &= \mathrm{e}^{\mathrm{i}\hat{H}t/\hbar} \\ &= \hat{U}(-t), \end{aligned} \tag{5.5}$$

from which it follows that

$$\begin{aligned} \hat{U}(t)^\dagger\hat{U}(t)\,|\psi(0)\rangle &= \hat{U}(t)^\dagger\,|\psi(t)\rangle \\ &= \hat{U}(-t)\,|\psi(t)\rangle \\ &= |\psi(0)\rangle\,, \end{aligned} \tag{5.6}$$

or in other words, $\hat{U}^\dagger\hat{U} = \hat{I}$, or $\hat{U}^\dagger = \hat{U}^{-1}$. Such an operator $\hat{A}$ that satisfies $\hat{A}^\dagger\hat{A} = \hat{I}$ is said to be *unitary*.

Let $\{|\psi_n\rangle\} \in \mathcal{H}$ be an eigenbasis of the Hamiltonian $\hat{H}$, i.e., $\hat{H}\,|\psi_n\rangle = \lambda_n\,|\psi_n\rangle$, where $\{\lambda_n\}_{n=0}^{\infty} \in \mathbb{R}$. We can expand the initial state in this basis as $|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n\,|\psi_n\rangle$, where $c_n = \langle\psi_n|\psi\rangle \in \mathbb{C}$, and thus write the state at time t as

$$\begin{aligned} |\psi(t)\rangle &= \mathrm{e}^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle \\ &= \left(\sum_{n=0}^{\infty} \frac{\left(-\mathrm{i}\hat{H}t/\hbar\right)^n}{n!}\right)\left(\sum_{m=0}^{\infty} c_m\,|\psi_m\rangle\right) \\ &= \sum_{m=0}^{\infty}\left(\sum_{n=0}^{\infty} c_m \frac{\left(-\mathrm{i}\hat{H}t/\hbar\right)^n}{n!}\,|\psi_m\rangle\right) \\ &= \sum_{m=0}^{\infty} \mathrm{e}^{-\mathrm{i}\lambda_m t/\hbar} c_m\,|\psi_m\rangle \\ &= \sum_{m=0}^{\infty} c_m \mathrm{e}^{-\mathrm{i}\lambda_m t/\hbar}\,|\psi_m\rangle\,. \end{aligned} \tag{5.7}$$

5.3 Case of temporally dependent Hamiltonian

Let now the Hamiltonian $\hat{H} = \hat{H}(t)$ be time-dependent. The Schrödinger equation still holds:

$$\mathrm{i}\hbar\partial_t |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle , \tag{5.8}$$

and the evolution is unitary. Thus $\exists\{\hat{U}(t)\} \in \mathcal{L}(\mathcal{H})$ s.t.

$$\hat{U}(t) |\psi(0)\rangle = |\psi(t)\rangle , \qquad \forall |\psi(t)\rangle \in \mathcal{H} \tag{5.9}$$

$$\Rightarrow \mathrm{i}\hbar\partial_t \left(\hat{U}(t) |\psi(0)\rangle\right) = \hat{H}(t) \left(\hat{U}(t) |\psi(0)\rangle\right) \tag{5.10}$$

$$\Rightarrow \mathrm{i}\hbar\partial_t\hat{U}(t) = \hat{H}(t)\hat{U}(t). \tag{5.11}$$

This is equivalent to the Schrödinger equation.

Exercise

Build $\hat{U}(t)$ for $\hat{H}(t)$.

5.4 Properties of unitary operators

For any two unitary operators $\hat{U}_1$ and $\hat{U}_2$, we have

$$\left(\hat{U}_1\hat{U}_2\right)^\dagger = \hat{U}_2^\dagger\hat{U}_1^\dagger = \hat{U}_2^{-1}\hat{U}_1^{-1} = \left(\hat{U}_1\hat{U}_2\right)^{-1} . \tag{5.12}$$

That is, $\hat{U}_1\hat{U}_2$ is also unitary.

Let $|\psi\rangle , |\phi\rangle \in \mathcal{H}$ and $\hat{U}^\dagger = \hat{U}^{-1} \in \mathcal{L}(\mathcal{H})$. We define

$$|\psi'\rangle = \hat{U} |\psi\rangle \quad \text{and} \quad |\phi'\rangle = \hat{U} |\phi\rangle , \tag{5.13}$$

for which we have

$$\begin{aligned} \langle\psi|\phi\rangle &= \langle\psi|\hat{I}|\phi\rangle = \langle\psi|\hat{U}^{-1}\hat{U}|\phi\rangle \\ &= \langle\psi|\hat{U}^\dagger\hat{U}|\phi\rangle = \left(\hat{U} |\psi\rangle , \hat{U} |\phi\rangle\right) \\ &= \langle\psi'|\phi'\rangle . \end{aligned} \tag{5.14}$$

Unitary operators can be considered as rotations.[2]

2: sometimes reflections as well

5.5 Qubit

A qubit can refer either to a physical system or to a mathematical construction. In either case, it is modeled by a a two-level quantum system as follows:

Let $\mathcal{H}_2 = \mathrm{span}\{|\tilde{0}\rangle, |\tilde{1}\rangle\}$, where $\langle\tilde{0}|\tilde{0}\rangle = 1 = \langle\tilde{1}|\tilde{1}\rangle$.

$\mathcal{H}_2$ fully describes all possible states of the qubit where

$$|\psi\rangle \in \mathcal{H}_2 \quad \text{and} \quad \| \, |\psi\rangle \, \| = 1. \tag{5.15}$$

Thus the qubit Hamiltonian $\hat{H}_q$ has just two eigenvalues $\varepsilon_1 \leq \varepsilon_2 \in \mathbb{R}$ and the corresponding eigenvectors are $|\mathrm{g}\rangle$ and $|\mathrm{e}\rangle$, respectively.[3]

3: Ground and excited

Thus,

$$\begin{aligned}
\hat{H}_q &= \varepsilon_1 |\mathrm{g}\rangle\langle \mathrm{g}| + \varepsilon_2 |\mathrm{e}\rangle\langle \mathrm{e}| \qquad (5.16)\\
&= \frac{\varepsilon}{2}\left(-|\mathrm{g}\rangle\langle \mathrm{g}| + |\mathrm{e}\rangle\langle \mathrm{e}|\right) + \frac{(\varepsilon_1+\varepsilon_2)}{2}|\mathrm{g}\rangle\langle \mathrm{g}| + \frac{(\varepsilon_1+\varepsilon_2)}{2}|\mathrm{e}\rangle\langle \mathrm{e}|\\
&= \frac{\varepsilon}{2}\left(-|\mathrm{g}\rangle\langle \mathrm{g}| + |\mathrm{e}\rangle\langle \mathrm{e}|\right) + \underbrace{\frac{\varepsilon_1+\varepsilon_2}{2}\hat{I}}_{\text{We can disregard this since it just equally changes the phase of all } |\psi\rangle \in \mathcal{H}_2}
\end{aligned}$$

where $\varepsilon = \varepsilon_2 - \varepsilon_1$.

Thus $\hat{H}_q = -\frac{\varepsilon}{2}\left(|\mathrm{g}\rangle\langle \mathrm{g}| - |\mathrm{e}\rangle\langle \mathrm{e}|\right)$.

We can define the qubit states $|0\rangle := |\mathrm{g}\rangle$ and $|1\rangle := |\mathrm{e}\rangle$.

Thus,

$$\begin{aligned}
\hat{H}_q &= -\frac{\varepsilon}{2}\hat{\sigma}_z, \qquad \hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \qquad (5.17)\\
&\mathrel{\hat{=}} \begin{bmatrix} -\frac{\varepsilon}{2} & 0 \\ 0 & +\frac{\varepsilon}{2} \end{bmatrix}.
\end{aligned}$$

The temporal evolution is given by

$$\begin{aligned}
|\psi(t)\rangle &= \mathrm{e}^{-\mathrm{i}\hat{H}_q t/\hbar}|\psi(0)\rangle, \qquad |\psi(0)\rangle = c_0|0\rangle + c_1|1\rangle \qquad (5.18)\\
&= \mathrm{e}^{+\mathrm{i}\frac{\varepsilon}{2}\hat{\sigma}_z t/\hbar}|\psi(0)\rangle\\
&= \mathrm{e}^{\mathrm{i}\frac{\varepsilon}{2}t/\hbar}c_0|0\rangle + \mathrm{e}^{-\mathrm{i}\frac{\varepsilon}{2}t/\hbar}c_1|1\rangle.
\end{aligned}$$

5.6 How to set up a qubit from a physical system

Very few physical systems are qubits. However, it is possible to take some physical systems and confine the dynamics to a subspace of two states. For example, a spin is a natural two-level system, but confined (for example in atoms). Another example is a non-linear system where $\varepsilon_0 < \varepsilon_1 < \varepsilon_2 \cdots$ are eigenvalues of $\hat{H}$ s.t. $\varepsilon_1 - \varepsilon_0 \neq \varepsilon_2 - \varepsilon_1$. See Fig. 5.1.

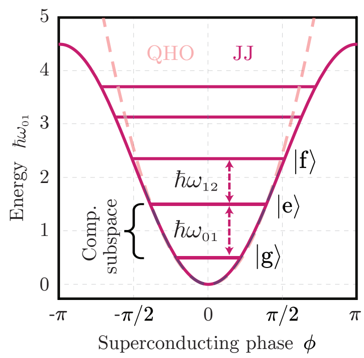

Figure 5.1: Non-linear harmonic oscillator with a Josephson junction (JJ). Notice that the gap $\hbar\omega_{01} \neq \hbar\omega_{12}$, i.e., the energy states are non-equidistant. Figure from Ref. [1].

5.7 Pauli operators

Definition 5.7.1 *The Pauli operators are*

$$\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \tag{5.19}$$
$$\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \tag{5.20}$$
$$\hat{\sigma}_y = -\mathrm{i}\,|0\rangle\langle 1| + \mathrm{i}\,|1\rangle\langle 0| \tag{5.21}$$

Properties

The Pauli operators have a number of interesting properties:

$$\hat{\sigma}_\alpha^2 = \hat{I} \qquad \forall\alpha \in \{\mathrm{x},\mathrm{y},\mathrm{z}\} \tag{5.22}$$
$$\hat{\sigma}_\alpha^\dagger = \hat{\sigma}_\alpha \qquad \forall\alpha \tag{5.23}$$
$$[\hat{\sigma}_i, \hat{\sigma}_j] = \sum_{k\in\{\mathrm{x},\mathrm{y},\mathrm{z}\}} 2\mathrm{i}\hat{\sigma}_k \varepsilon_{ijk}, \qquad \forall i,j \in \{\mathrm{x},\mathrm{y},\mathrm{z}\}, \tag{5.24}$$

where

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \in \{(\mathrm{x},\mathrm{y},\mathrm{z}), (\mathrm{z},\mathrm{x},\mathrm{y}), (\mathrm{y},\mathrm{z},\mathrm{x})\}, \\ -1 & \text{if } (i,j,k) \in \{(\mathrm{y},\mathrm{x},\mathrm{z}), (\mathrm{z},\mathrm{y},\mathrm{x}), (\mathrm{x},\mathrm{z},\mathrm{y})\}, \\ 0 & \text{otherwise,} \end{cases} \tag{5.25}$$

is the Levi-Civita symbol.

Definition 5.7.2

$$\hat{\sigma}^- = |0\rangle\langle 1| \tag{5.26}$$
$$\hat{\sigma}^+ = (\hat{\sigma}^-)^\dagger = |1\rangle\langle 0|\,. \tag{5.27}$$

Exercise

Show that

$$e^{\mathrm{i}\varphi\vec{a}\cdot\hat{\vec{\sigma}}} = \hat{I}\cos\varphi + \mathrm{i}\;\vec{a}\cdot\hat{\vec{\sigma}}\sin\varphi,$$

where $\vec{a} \in \mathbb{R}^3$, $||\vec{a}|| = 1$ and $\vec{a}\cdot\hat{\vec{\sigma}} = a_\mathrm{x}\hat{\sigma}_\mathrm{x} + a_\mathrm{y}\hat{\sigma}_\mathrm{y} + a_\mathrm{y}\hat{\sigma}_\mathrm{z}$.

5.8 Bloch sphere

Definition 5.8.1 *A qubit state can always be expressed as*

$$|\psi\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{\mathrm{i}\varphi}\sin\frac{\theta}{2}\,|1\rangle\,, \tag{5.28}$$

where φ is the azimuthal angle and θ is the polar angle.

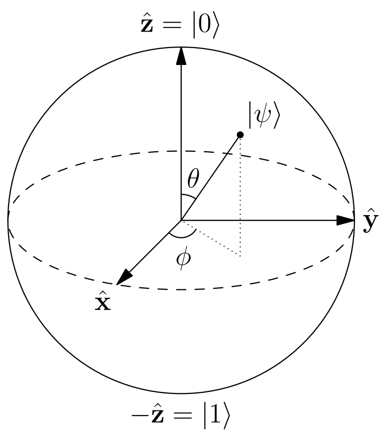

Figure 5.2: Bloch sphere representation [2].

Note that since a global phase of the state $e^{i\alpha}$ does not affect any measurement outcome, i.e.,

$$\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}e^{-i\alpha}e^{i\alpha}|\psi\rangle = \langle\psi|e^{-i\alpha}\hat{A}e^{i\alpha}|\psi\rangle = \langle e^{i\alpha}\psi|\hat{A}e^{i\alpha}|\psi\rangle\,, \tag{5.29}$$

we can always choose $c_0 \in \mathbb{R}$ in $|\psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle$.

Thus, for each state there are unique $\theta \in [0, \pi)$ and $\varphi \in [0, 2\pi)$ which correspond to a point on a unit sphere as shown in Fig. 5.2.

Exercise

Show that $\hat{U}(t)$ are rotations of the Bloch vectors.

Lecture 6 | 6

Last lecture from Mikko.

6.1 Intended learning outcomes

- Apply tensor product to construct a quantum register of N qubits
- Identify the constituents of a quantum algorithm
- Apply the commutator to identify conserved quantities

6.2 Tunable Hamiltonian for quantum gates

Let span $\{|0\rangle, |1\rangle\} = \mathcal{H}_2$ and assume that control over the Hamiltonian s.t. $\hat{H} = \varepsilon_0 \vec{a}(t) \cdot \hat{\vec{\sigma}}$, where $\vec{a} \in \mathbb{R}^3$, $\|\vec{a}\| = 1$, and $\varepsilon_0 \in \mathbb{R}$ has units of energy.

Thus any unitary evolution[1] $\hat{U} = \hat{I}\cos\theta + \mathrm{i}\,\vec{b} \cdot \hat{\vec{\sigma}} \sin\theta$ can be implemented, for example, by a control sequence

1: An unitary operation on a qubit is referred to as a single-qubit gate

$$\vec{a}(t) = \begin{cases} 0, & t < 0 \\ -\varepsilon_0 \vec{b}, & 0 \le t \le \theta\hbar/\varepsilon_0 \\ 0, & \theta\hbar/\varepsilon_0 < t \end{cases} . \tag{6.1}$$

There are many other ways of course. Note that there is also a way to use

$$\hat{H} = -\frac{\varepsilon}{2}\hat{\sigma}_z \tag{6.2}$$

and apply a field $\vec{H}_{ex}(t) = \frac{\Omega}{2}\hat{\sigma}_x \sin(\omega t + \phi)$, where $\omega = \frac{\varepsilon}{\hbar}$. That will result in so-called Rabi oscillations to be discussed later.

6.3 Single-qubit gates: examples

- The NOT gate corresponds to $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \mathrel{\hat{=}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.
- Hadamard gate corresponds to $\hat{H}_g = \frac{1}{\sqrt{2}}(\hat{\sigma}_x + \hat{\sigma}_z) \mathrel{\hat{=}} \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$.
- Phase flip corresponds to $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \mathrel{\hat{=}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.

Exercise

Find $\hat{a}(t)$ implementing:

$$\hat{H}_g \hat{\sigma}_x \hat{H}_g = \hat{\sigma}_z$$
$$\hat{H}_g^\dagger = \hat{H}_g = \hat{H}_g^{-1}.$$

6.4 Qubit measurement

Let $|\psi\rangle \in \mathcal{H}_2$ be a qubit state. Thus we may write $|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle$, where $c_0, c_1 \in \mathbb{C}$ s.t. $|c_0|^2 + |c_1|^2 = 1$. Thus the measurement probabilities are given by

$$P_0 = |\langle 0|\psi\rangle|^2 = |c_0|^2 \tag{6.3}$$
$$P_1 = |\langle 1|\psi\rangle|^2 = |c_1|^2 = 1 - |c_0|^2 \tag{6.4}$$

After applying a quantum gate $\hat{U}$ on $|\psi\rangle$ the probabilities are given by

$$P_0 = \left|\langle 0|\hat{U}|\psi\rangle\right|^2 = \langle\psi|\hat{U}^\dagger|0\rangle\langle 0|\hat{U}|\psi\rangle = \left|\langle\tilde{0}|\psi\rangle\right|^2, \tag{6.5}$$

where $|\tilde{0}\rangle = \hat{U}^\dagger |0\rangle$. Similarly for $P_1 = \left|\langle 1|\hat{U}|\psi\rangle\right|^2 = \left|\langle\tilde{1}|\psi\rangle\right|^2$.

6.5 2-qubit system

The Hilbert space $\mathcal{H}_4 = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)}$ of a system composed of two qubits is 4-dimensional. The symbol $\otimes$ denotes the tensor product of Hilbert spaces or vectors. Single-qubit operators are of the form $\hat{A}_1 \otimes \hat{I}$ and $\hat{I} \otimes \hat{A}_2$, where $\hat{A}_1 \in \mathcal{L}(\mathcal{H}_2^{(1)})$ and $\hat{A}_2 \in \mathcal{L}(\mathcal{H}_2^{(2)})$.

On the tensor product

The tensor product (or Kronecker product) is a bilinear composition of the two vector spaces (with minimal constraints).

Let $\hat{A} \otimes \hat{B} = \hat{C} \in \mathcal{L}(\mathcal{H}_4)$ and $\hat{D} \otimes \hat{E} = \hat{F} \in \mathcal{L}(\mathcal{H}_4)$. From the properties of the tensor product, it follows that

$$\hat{C}\hat{F} = \left(\hat{A} \otimes \hat{B}\right)\left(\hat{D} \otimes \hat{E}\right) = \left(\hat{A}\hat{D}\right) \otimes \left(\hat{B}\hat{E}\right). \tag{6.6}$$

Definition 6.5.1 *We construct the basis for the two-qubit Hilbert space $\mathcal{H}_4$ as*

$$|00\rangle := |0\rangle \otimes |0\rangle \tag{6.7}$$
$$|01\rangle := |0\rangle \otimes |1\rangle \tag{6.8}$$
$$|10\rangle := |1\rangle \otimes |0\rangle \tag{6.9}$$
$$|11\rangle := |1\rangle \otimes |1\rangle, \tag{6.10}$$

where $\{|0\rangle, |1\rangle\}$ *is an orthonormal basis for* $\mathcal{H}_2^{(1)}$ *and* $\mathcal{H}_2^{(2)}$*, respectively.*

Thus for $|\psi\rangle \in \mathcal{H}_4$, we may write

$$\begin{aligned} |\psi\rangle &= \sum_{k=0}^{3} c_k |k\rangle \qquad (6.11) \\ &= c_0 |00\rangle + c_1 |01\rangle + c_2 |10\rangle + c_3 |11\rangle \\ &= c_0 |0\rangle + c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle \end{aligned}$$

where $|k\rangle := |k_1 k_2\rangle$, where $k_1 k_2$ is a binary representation of k.

Additionally, for $\hat{C} = \hat{A} \otimes \hat{B} \in \mathcal{L}(\mathcal{H}_4)$, we have

$$\begin{aligned} \hat{C} |\psi\rangle = \hat{C} \sum_{k=0}^{3} c_k |k\rangle &= \sum_{k=0}^{3} c_k \hat{C} |k\rangle \qquad (6.12) \\ &= \sum_{k=0}^{3} c_k \hat{A} \otimes \hat{B} \underbrace{|k\rangle}_{\in \mathcal{H}_4} \\ &= \sum_{k=0}^{3} c_k \hat{A} \underbrace{|k_1\rangle}_{\in \mathcal{H}_2^{(1)}} \otimes \hat{B} \underbrace{|k_2\rangle}_{\in \mathcal{H}_2^{(2)}} . \end{aligned}$$

6.6 Examples of two-qubit gates

Controlled NOT (CNOT) gate where qubit 1 is the control qubit and qubit 2 is the target qubit corresponds to

$$\begin{aligned} \hat{C}_{\text{NOT}}^{(1,2)} &= |0\rangle\langle 0| \otimes \hat{I} + |1\rangle\langle 1| \otimes \hat{\sigma}_x \qquad (6.13) \\ &\hat{=} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & \sigma_x \end{bmatrix} . \end{aligned}$$

Exercise

- Construct the above matrix representations
- Express CNOT that has qubit 1 as the target qubit

6.7 n-qubit system

For a system with n qubits, we usually define $N := 2^n = \dim\{\mathcal{H}_{2^n}\}$, and we have the following properties:

- $\mathcal{H}_{2^n} = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)} \otimes \cdots \otimes \mathcal{H}_2^{(n)}$
- $|\psi\rangle = \sum_{k=0}^{2^n-1} c_k |k\rangle = c_0 |\underbrace{00\cdots0}_{n \text{ zeroes}}\rangle + c_1 |\underbrace{0\cdots0}_{n-1 \text{ zeroes}}1\rangle + \cdots$, where again $|k\rangle$ means $|k_1 k_2 \ldots k_n\rangle$, where $k_1 k_2 \ldots k_n$ is k written in binary
- $\underbrace{\hat{I} \otimes \cdots \otimes \hat{I}}_{m-1} \otimes \hat{A} \otimes \underbrace{\hat{I} \otimes \cdots \otimes \hat{I}}_{n-m}$ is a single-qubit operator for qubit m.

6.8 Quantum algorithms for n qubits

In general, a *quantum algorithm* is a procedure consisting of the following steps:

1. Initialize qubits to $|0\rangle$.[2]
2. Apply a desired n-qubit gate $\mathbf{U}$.[3]
3. Measure qubits.[4]
4. Use measurement data and go to 1, unless algorithm finished.[5]

2: Not necessarily all qubits

3: Can be constructed from single and two-qubit gates

4: Not necessarily all qubits

5: In the simplest case one goes only once through 1. → 4. and initializes and measures all qubits in 1. and 3., respectively.

Exercise

Deustch algorithm

6.9 Entanglement for two qubits

Definition 6.9.1 *A quantum state of two qubits is defined to be entangled iff it cannot be represented as a product of two single-qubit states.*

Thus $\forall |\psi\rangle \in \mathcal{H}_4$ that are not entangled $\exists |\psi_1\rangle \in \mathcal{H}_2^{(1)}$ and $|\psi_2\rangle \in \mathcal{H}_2^{(2)}$ s.t.

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \tag{6.14}$$

Examples of so-called maximally entangled states are *Bell states*

$$|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle) \tag{6.15}$$

$$|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle) \tag{6.16}$$

6.10 Commuting operators

Let $\hat{A}, \hat{B} \in \mathcal{L}(\mathcal{H})$ be Hermitian operators with $[\hat{A}, \hat{B}] = 0$. In this case, it can be shown that there exists a complete eigenbasis of $\hat{A}$ that is also an eigenbasis of $\hat{B}$.

Especially if $[\hat{A}, \hat{H}(t)] = 0$, $\forall t$, the eigenvalues of $\hat{A}$ are referred to as conserved quantities since we have

$$\begin{aligned} \hat{A} |\psi(t)\rangle &= \hat{A}\hat{U}(t) |\psi(0)\rangle = \hat{U}(t)\hat{A} |\psi(0)\rangle \\ &= \lambda\hat{U}(t) |\psi(0)\rangle = \lambda |\psi(t)\rangle , \end{aligned} \tag{6.17}$$

where we have assumed that $\hat{A} |\psi(0)\rangle = \lambda |\psi(0)\rangle$, i.e., we start from an eigenstate of $\hat{A}$.

References

[1] Niko Savola. *Electromagnetic simulation of superconducting qubit–resonator coupling*. English. Bachelor's Thesis. 2020. URL: http://urn.fi/URN:NBN:fi:aalto-202009155417 (cited on page 26).

[2] Wikimedia Commons. *File:Bloch Sphere.svg — Wikimedia Commons, the free media repository*. [Online; accessed 5th August 2021]. 2020. URL: %5Curl%7Bhttps://commons.wikimedia.org/w/index.php?title=File:Bloch_Sphere.svg&oldid=514662857%7D (cited on page 27).