PHYS-C0252 - Quantum Mechanics 2024

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 constructions 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 study such advanced mathematics in the Master-level courses to fill in the gaps not bridged in this course. To keep you on track, we intend to tell you when we do not prove or discuss something rigorously.

Quantum mechanics is delicious. Enjoy!

1.3 Hilbert space and ket 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.

Math on complex conjugation

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

$$z = x + \mathrm{i}y$$
$$z^* = x - \mathrm{i}y$$

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

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 $|f(v)| \leq M\|v\|$.

so-called Riesz representation theorem[3] states that for any linear 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 $\mathcal{H}$.

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

1.5 Linear operators

Definition 1.5.1 *A mapping $\hat{A}$ is a linear operator on $\mathcal{H}$* $\iff$ $\hat{A} : \mathcal{H} \to \mathcal{H}$ *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.

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2.1 Intended learning outcomes

- Use bases to represent vectors and operators
- Differentiate between a quantum state and its representation as a column vector.
- Identify useful properties of Hermitian operators.

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 coordinates for them using a basis.

Definition 2.2.1 *A set of ket vectors* $\{|\phi_i\rangle\}_{i=1}^N \subset \mathcal{H}$, $N \in \mathbb{Z}_+$, *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 $\{|\phi_i\rangle\}_{i=1}^N \subset \mathcal{H}$ 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 $|\phi_k\rangle$. 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* $\mathcal{H}$.

The coefficients c_k are the *coordinates* of $|\psi\rangle$ *with respect to the basis spanned by* $\{\phi_k\}$.

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

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

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

In other words, we can express the coefficient c_k of the kth component of $|\psi\rangle$ in the basis $|\phi_k\rangle$ as $\langle\phi_k|\psi\rangle$. Plugging this into the right hand side of Eq. (2.2), we find

$$\begin{aligned} |\psi\rangle &= \sum_k \langle\phi_k|\psi\rangle|\phi_k\rangle \\ &= \sum_k |\phi_k\rangle\langle\phi_k|\psi\rangle \\ &= \left(\sum_k |\phi_k\rangle\langle\phi_k|\right)|\psi\rangle\,, \end{aligned} \tag{2.4}$$

where in the last step, we have used the fact that the outer product is linear. Based on this, we conclude that $\sum_k |\phi_k\rangle\langle\phi_k| = \hat{I}$, the identity operator. Importantly, 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

$$|\psi\rangle = \sum_k c_k \, |\phi_k\rangle \tag{2.5}$$

$$\hat{=} \underbrace{\begin{bmatrix} c_1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}}_{c_1|\phi_1\rangle} + \underbrace{\begin{bmatrix} 0 \\ c_2 \\ 0 \\ \vdots \end{bmatrix}}_{c_2|\phi_2\rangle} + \underbrace{\begin{bmatrix} 0 \\ 0 \\ c_3 \\ \vdots \end{bmatrix}}_{c_3|\phi_3\rangle} + \cdots = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix},$$

where $\hat{=}$ stands for *represented by*. In a given basis, 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 $|\psi\rangle$:

$$\langle\psi| \hat{=} \begin{bmatrix} c_1^* & c_2^* & c_3^* & \dots \end{bmatrix}. \tag{2.6}$$

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,

$$\begin{aligned}\hat{A} = \hat{I}\hat{A}\hat{I} &= \left(\sum_m |\phi_m\rangle\langle\phi_m|\right)\hat{A}\left(\sum_k |\phi_k\rangle\langle\phi_k|\right) \qquad (2.7)\\ &= \sum_{m,k} |\phi_m\rangle \underbrace{\langle\phi_m|\hat{A}|\phi_k\rangle}_{:=A_{mk}\in\mathbb{C}} \langle\phi_k| \\ &= \sum_{m,k} A_{mk}\,|\phi_m\rangle\langle\phi_k| \\ &\hat{=} \begin{bmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}.\end{aligned}$$

This is the *matrix representation* of the operator $\hat{A}$ in this basis. The matrix element at row m and column k is given by $A_{mk} = \langle\phi_m|\hat{A}|\phi_k\rangle$. Note that the matrix might be infinite-dimensional.

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

$$\begin{aligned}\hat{A}\,|\psi\rangle &= \sum_{m,k,l} A_{mk}\,|\phi_m\rangle\langle\phi_k|c_l|\phi_l\rangle \qquad (2.8)\\ &= \sum_{m,k,l} A_{mk}c_l\,|\phi_m\rangle \underbrace{\langle\phi_k|\phi_l\rangle}_{=\delta_{kl}} \qquad (2.9)\\ &= \sum_{m,k} A_{mk}c_k\,|\phi_m\rangle\,.\end{aligned}$$

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

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

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 $|\psi\rangle$.

2.5 Adjoint

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

$$\left(\langle\phi| \, \hat{A}\right) |\psi\rangle = \langle\phi| \left(\hat{A} \, |\psi\rangle\right). \tag{2.10}$$

2: An operator $\hat{A}$ is defined to be bounded if there exists a constant $M > 0$ such that $\forall \, |\psi\rangle \in \mathcal{H}$ we have $\|\hat{A} \, |\psi\rangle \| \leq M \| \, |\psi\rangle \|$.

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

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

$$\hat{A}^\dagger \, |\phi\rangle = |\phi'\rangle, \tag{2.11}$$

which is referred to as the *adjoint* of $\hat{A}$. The symbol † is pronounced "dagger", and $\hat{A}^\dagger$ is pronounced "A dagger".

About notation

These are equivalent:

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

The dagger notation is also used to denote the bra vector corresponding to a given ket vector: $(|\psi\rangle)^\dagger = \langle\psi|$ and similarly $(\langle\psi|)^\dagger = |\psi\rangle$.

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

$$\begin{aligned} \langle\phi|c|\psi\rangle &= \left(|\phi\rangle, c \, |\psi\rangle\right) \\ &= c \left(|\phi\rangle, |\psi\rangle\right) \\ &= \left(c^* \, |\phi\rangle, |\psi\rangle\right), \end{aligned} \tag{2.12}$$

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

As another example, consider the operator and ket vectors represented by the following matrix and vectors:

$$\hat{A} \doteq \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad |\phi\rangle \doteq \begin{bmatrix} x \\ y \end{bmatrix}, \quad |\psi\rangle \doteq \begin{bmatrix} u \\ v \end{bmatrix}, \tag{2.13}$$

where a, b, c, d, x, y, u, v are complex numbers. So, what is the matrix representation of $\hat{A}^\dagger$? We know that

$$\hat{A} \, |\psi\rangle \doteq \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix}. \tag{2.14}$$

Using Eq. (2.10) and the Riesz representation theorem, we know there must exist some vector

$$|\phi'\rangle \doteq \begin{bmatrix} z \\ w \end{bmatrix} \tag{2.15}$$

that satisfies

$$\langle \phi' | = \langle \phi | \hat{A} \mathrel{\hat{=}} \begin{bmatrix} z^* & w^* \end{bmatrix}. \tag{2.16}$$

Using the definition of the inner product, we have[3]

$$\begin{aligned} \langle \phi | \hat{A} | \psi \rangle &= \left(|\phi\rangle, \hat{A} |\psi\rangle \right) && (2.17) \\ &= \left(\begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix} \right) \\ &= \begin{bmatrix} x^* & y^* \end{bmatrix} \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix} && (2.18) \\ &= x^*(au + bv) + y^*(cu + dv). \end{aligned}$$

3: Note that here we use the regular equals symbol instead of $\hat{=}$. The inner product is just a number, which is equal for both the matrix/vector and abstract operator/ket vector representations.

But on the other hand

$$\begin{aligned} \langle \phi | \hat{A} | \psi \rangle &= \langle \phi' | \psi \rangle && (2.19) \\ &= \begin{bmatrix} z^* & w^* \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} \\ &= z^* u + w^* v, \end{aligned}$$

which means that

$$\begin{aligned} z^* u + w^* v &= x^*(au + bv) + y^*(cu + dv) && (2.20) \\ &= (x^* a + y^* c)u + (x^* b + y^* d)v \end{aligned}$$

$$\Rightarrow z = (x^* a + y^* c)^* = x a^* + y c^* \tag{2.21}$$

$$w = (x^* b + y^* d)^* = x b^* + y d^*. \tag{2.22}$$

From Eq. (2.11), it follows that the matrix representation of $\hat{A}^\dagger$ should be a matrix $A^\dagger$ that satisfies

$$\hat{A}^\dagger |\phi\rangle = |\phi'\rangle \mathrel{\hat{=}} A^\dagger \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} z \\ w \end{bmatrix} = \begin{bmatrix} x a^* + y c^* \\ x b^* + y d^* \end{bmatrix}. \tag{2.23}$$

We can clearly see that this matrix is

$$A^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix} = \left(\begin{bmatrix} a & b \\ c & d \end{bmatrix}^T \right)^*. \tag{2.24}$$

In other words, the matrix representation of the adjoint $\hat{A}^\dagger$ is the conjugate transpose of the matrix representation of $\hat{A}$, which is obtained by taking the transpose and then conjugating each element. While the above is not a rigorous proof, this holds in general.

2.6 Properties of adjoint

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

$$\left(\hat{A}^\dagger\right)^\dagger = \hat{A}, \tag{2.25}$$

$$\left(a\hat{A}\right)^\dagger = a^*\hat{A}^\dagger, \qquad (a \in \mathbb{C}), \tag{2.26}$$

$$\left(\hat{A}+\hat{B}\right)^\dagger = \hat{A}^\dagger + \hat{B}^\dagger, \tag{2.27}$$

$$\left(\hat{A}\hat{B}\right)^\dagger = \hat{B}^\dagger\hat{A}^\dagger, \tag{2.28}$$

$$\left(|\psi\rangle\langle\phi|\right)^\dagger = |\phi\rangle\langle\psi|, \tag{2.29}$$

$$\left(a\,|\psi\rangle\right)^\dagger = \langle\psi|\,a^* = a^*\,\langle\psi|, \qquad (a \in \mathbb{C}), \tag{2.30}$$

$$\left(\hat{A}\,|\psi\rangle\right)^\dagger = \langle\psi|\,\hat{A}^\dagger. \tag{2.31}$$

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*

$$\hat{A}\,|\psi_k\rangle = \lambda_k\,|\psi_k\rangle \tag{2.32}$$

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. (2.32), with $i = 1, \ldots, g_k$. 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*[4] $\hat{H}^\dagger = \hat{H}$.

4: 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

$$\hat{H}\,|\psi_k\rangle = \lambda_k\,|\psi_k\rangle\,. \tag{2.33}$$

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

$$\hat{H} = \sum_k \lambda_k\,|\psi_k\rangle\langle\psi_k|\,. \tag{2.34}$$

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.

Lecture 3 | 3

3.1 Intended learning outcomes

- Identify the minimal mathematical structure to describe a physical system quantum mechanically
- Differentiate between a measurement outcome and its expectation value
- Identify the Robertson uncertainty relation

3.2 Postulates of quantum mechanics

Finally, we 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)[1] Hilbert space.

1: What rigged means, will not be asked in the exam. We discuss it very briefly 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 $\hat{A}$.[2]

2: 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 $\mathcal{H}$, $\{|\phi_{n,i}\rangle\}_{n,i=\in\{1,\dots,g_n\}}$, 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

$$P(a_n) \coloneqq \sum_{i=1}^{g_n} \left|\langle\phi_{n,i}|\psi\rangle\right|^2 . \tag{3.1}$$

Note that if the state is multiplied by a phase factor $e^{i\varphi}$, the measurement probabilities are unaffected: If we replace $|\psi\rangle$ by $e^{i\varphi}|\psi\rangle$ in Eq. (3.1), we get the exact same result:

$$\sum_{i=1}^{g_n} \left|\langle\phi_{n,i}|e^{i\varphi}|\psi\rangle\right|^2 = \sum_{i=1}^{g_n} \underbrace{|e^{i\varphi}|^2}_{=1} \left|\langle\phi_{n,i}|\psi\rangle\right|^2 = P(a_n). \tag{3.2}$$

This is why a global phase offset cannot be measured.

Phase factor

A complex number $e^{i\varphi}$ with $\varphi \in \mathbb{R}$ is called a *phase factor*, because multiplying any complex number by it just shifts the phase (i.e. argument, or angle) of that number by φ. A phase factor has unit magnitude:

$$\left|e^{i\varphi}\right| = 1 \quad \forall\varphi.$$

See the Brief Summary for more details.

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

$$|\psi'\rangle = \frac{\hat{P}_n|\psi\rangle}{\|\hat{P}_n|\psi\rangle\|}, \qquad \hat{P}_n = \sum_{i=1}^{g_n} |\phi_{n,i}\rangle\langle\phi_{n,i}| . \tag{3.3}$$

$\hat{P}_n$ 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 3.2.1 *$\hat{P}_n \in \mathcal{L}(\mathcal{H})$ 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 *time-dependent Schrödinger equation*:

$$i\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle , \tag{3.4}$$

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.[3]

3: 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., $\hat{H} = \hat{H}[\alpha_1(t), \alpha_2(t), \dots]$. This is discussed later.

3.3 Expectation values

Definition 3.3.1 *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*

$$\langle \hat{A} \rangle_\psi = \langle \hat{A} \rangle := \langle \psi | \hat{A} | \psi \rangle . \tag{3.5}$$

This definition is valid for any linear operator $\hat{A}$. However, it is particularly interesting when $\hat{A}$ is Hermitian, with a corresponding observable quantity A. In this case, 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

$$\begin{aligned}
\langle \psi | \hat{A} | \psi \rangle &= \left(\sum_k c_k |\phi_k\rangle \right)^\dagger \hat{A} \sum_k c_k |\phi_k\rangle \\
&= \left(\sum_k c_k |\phi_k\rangle \right)^\dagger \sum_k c_k a_k |\phi_k\rangle \\
&= \sum_{n,k} c_n^* a_k c_k \langle \phi_n | \phi_k \rangle \\
&= \sum_k a_k \underbrace{|c_k|^2}_{P(a_k)} = \sum_k a_k P(a_k).
\end{aligned} \tag{3.6}$$

The sum on the right side of the last equality above is the classical definition of the expectation value for the measurement outcomes. It is important to note that the involved probabilities $P(a_k)$ arise from quantum mechanics. Even if a system is completely deterministically prepared in some state, the measurement outcomes will follow some probability distribution. This is not the same as preparing the system probabilistically in some state.[4]

4: Probabilistically prepared quantum states can be described by the so-called *density operator formalism*, which is discussed below.

3.4 Variance

Definition 3.4.1 *We define the variance of $\hat{A}$ when the system is in the state $|\psi\rangle$ as*

$$\begin{aligned}\Delta A^2 &= \langle\psi|\left(\hat{A} - \langle\psi|\hat{A}|\psi\rangle\right)^2|\psi\rangle \\ &= \langle\psi|\hat{A}^2|\psi\rangle - \left(\langle\psi|\hat{A}|\psi\rangle\right)^2 \\ &= \sum_k a_k^2 P(a_k) - \left(\sum_k a_k P(a_k)\right)^2 .\end{aligned} \tag{3.7}$$

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.

Powers of operators

An operator raised to a power just means repeatedly applying the operator:

$$\hat{A}^n = \underbrace{\hat{A}\hat{A}\cdots\hat{A}}_{\text{Repeated } n \text{ times}}.$$

For example, $\hat{A}^2|\psi\rangle = \hat{A}\hat{A}|\psi\rangle$.

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 Robertson uncertainty relation

Although the above definitions of the mean and variance of quantum-measurement results are in agreement with the corresponding classical definitions, the fact that these measurement results stem from a quantum system may have a profound effect on the outcomes. Such an effect is vested in the famous Heisenberg uncertainty relation which we introduce on the next lecture. At this point, however, we are ready to prove another uncertainty relation, namely, the Robertson uncertainty relation that yields the Heisenberg uncertainty relation as a spacial case.

Definition 3.6.1 *The Robertson uncertainty relation is defined as*

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle[\hat{A}, \hat{B}]\rangle\right|, \tag{3.8}$$

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

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,

$$\begin{aligned}\Delta A^2 &= \langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\right)^2|\psi\rangle \\ &= \underbrace{\langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)}_{\left(\left(\hat{A}-\langle\hat{A}\rangle\hat{I}\right)|\psi\rangle\right)^\dagger}\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)|\psi\rangle \\ &= \langle f|f\rangle = \||f\rangle\|^2,\end{aligned} \tag{3.9}$$

Math on norm of $\mathbb{C}$

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

$$\begin{aligned}|z|^2 &= (\mathrm{Re}\ z)^2 + (\mathrm{Im}\ z)^2 \\ &\geq (\mathrm{Im}\ z)^2 = \left(\frac{z - z^*}{2\mathrm{i}}\right)^2\end{aligned}$$

and similarly,

$$\Delta B^2 = \langle g|g\rangle = \||g\rangle\|^2. \tag{3.10}$$

Then, the Cauchy–Schwarz inequality implies

$$|\langle f|g\rangle| \leq \||f\rangle\|\,\||g\rangle\| \tag{3.11}$$

$$\begin{aligned}\Rightarrow \Delta A^2 \Delta B^2 &\geq |\underbrace{\langle f|g\rangle}_{\in\mathbb{C}}|^2 \\ &= \left|\langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)\left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)|\psi\rangle\right|^2 \\ &\geq \frac{\left|\langle\psi|\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)\left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)|\psi\rangle - \langle\psi|\left(\hat{B} - \langle\hat{B}\rangle\hat{I}\right)\left(\hat{A} - \langle\hat{A}\rangle\hat{I}\right)|\psi\rangle\right|^2}{4} \\ &= \frac{\left|\langle\psi|[\hat{A} - \langle\hat{A}\rangle\hat{I}, \hat{B} - \langle\hat{B}\rangle\hat{I}]|\psi\rangle\right|^2}{4} \\ &= \frac{\left|\langle[\hat{A}, \hat{B}]\rangle\right|^2}{4} \quad \square\end{aligned} \tag{3.12}$$

Lecture 4 | 4

4.1 Intended learning outcomes

- Apply Lagrangian formalism to quantize physical systems
- Apply canonical commutation relations
- Apply creation and annihilation operators for a harmonic oscillator
- Identify Heisenberg's uncertainty relation

4.2 On modeling a quantum-mechanical system

In the previous chapter, we introduced how to connect the mathematical formalism of quantum mechanics to physics through the postulates of quantum mechanics. One may use this formalism to describe possible measurement results and probabilities of physically measurable quantities, solve the temporal evolution of the system, and hence find out how to prepare the system to a certain initial state or even design the system to carry out certain desired dynamics.

Because the eigenstates of the Hamiltonian provide us a representation of the relevant Hilbert space and can be used to determine the temporal evolution of the system, finding these eigenstates leads to enough information to fully solve the physics of the system. The set of possible measurement results of the energy, i.e., the set of eigenvalues of the Hamiltonian, is defined as the *energy spectrum* of the system. Just the *spectrum* refers to the set of eigenvalues of any corresponding operator.

4.3 Classical pendulum

Above, we have stressed the importance of the Hamiltonian, but how do we obtain the Hamiltonian of a given 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, we provide a general procedure, or recipe, for converting the classical

Hamiltonian of any system to the corresponding quantum Hamiltonian. Later, we use the obtained Hamiltonian for the pendulum to describe the quantum harmonic oscillator.

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. 4.1. 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

$$q = l\theta. \tag{4.1}$$

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

$$\begin{aligned} V &= gmh \\ &= mgl\,(1-\cos\theta) \approx \frac{1}{2}mgl\theta^2 = \frac{mg}{2l}q^2. \end{aligned} \tag{4.2}$$

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

$$T = \frac{1}{2}mv^2 = \frac{1}{2}ml^2\dot{\theta}^2 = \frac{1}{2}m\dot{q}^2. \tag{4.3}$$

Definition 4.3.1 *The* Lagrangian *is defined as*

$$L \coloneqq T - V. \tag{4.4}$$

Thus, the Lagrangian for our case is

$$\begin{aligned} L = T - V &= \frac{1}{2}ml^2\dot{\theta}^2 - \frac{1}{2}mgl\theta^2 \\ &= \frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2. \end{aligned} \tag{4.5}$$

Definition 4.3.2 *The* generalized momentum *corresponding to the*

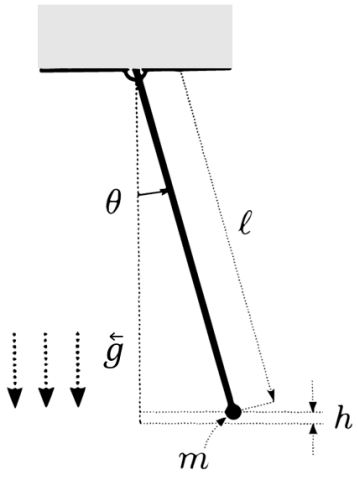

Figure 4.1: Ideal classical pendulum, where a mass m is attached to a massless rigid rod of length l. The rod may rotate without friction about a single axis as described by the angle θ. We assume a uniform gravitational field described by g.

Math on dot notation

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

Math on Taylor series

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

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)

$$p = \frac{\partial}{\partial \dot{q}} \left(\frac{1}{2} m \dot{q}^2 - \frac{mg}{2l} q^2 \right) = m\dot{q}. \tag{4.6}$$

Definition 4.3.3 *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):

$$\begin{aligned} H &= \dot{q}p - L = m\dot{q}^2 - \left(\frac{1}{2} m \dot{q}^2 - \frac{mg}{2l} q^2 \right) \\ &= \frac{p^2}{2m} + \frac{mg}{2l} q^2 = T + V. \end{aligned} \tag{4.7}$$

4.4 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:** The positions and momenta must satisfy $[\hat{p}_i, \hat{q}_i] = \hat{p}_i\hat{q}_i - \hat{q}_i\hat{p}_i = -\mathrm{i}\hbar$, 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 $\mathrm{i}\hbar\partial_t |\psi\rangle = \hat{H} |\psi\rangle$.

For the pendulum discussed above, the quantization procedure simply yields

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mg}{2l}\hat{q}^2. \tag{4.8}$$

The significance of the CCR and the temporal evolution for the harmonic oscillator will be discussed later.

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.[1] Another important application is the quantization of the electromagnetic Ffield, which follows a similar procedure but with a continuous set of generalized coordinates.

1: This is discussed in the Quantum Circuits course.

4.5 One-dimensional quantum harmonic oscillator

As we derived above in Eq. (4.8), the operator corresponding to the classical Hamiltonian of the harmonic oscillator is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\underbrace{\frac{g}{l}}_{=:\omega^2}\hat{q}^2 \tag{4.9}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \tag{4.10}$$

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 $A, B, C \in \mathbb{R}$:

$$\hat{H} = (A\hat{q} - \mathrm{i}B\hat{p})\,(A\hat{q} + \mathrm{i}B\hat{p}) + C. \tag{4.11}$$

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

Math on $\mathbb{C}$

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

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

find

$$\begin{aligned}\hat{H} &= A^2\hat{q}^2 + \mathrm{i}AB\hat{q}\hat{p} - \mathrm{i}B\hat{p}A\hat{q} + B^2\hat{p}^2 + C \\ &= A^2\hat{q}^2 + B^2\hat{p}^2 + \underbrace{\mathrm{i}AB\underbrace{[\hat{q},\hat{p}]}_{=\mathrm{i}\hbar}}_{=-\hbar AB} + C.\end{aligned} \tag{4.12}$$

Comparing this to Eq. (4.10), we choose

$$A = \sqrt{\frac{1}{2}m\omega^2}, \tag{4.13}$$

$$B = \sqrt{\frac{1}{2m}}, \tag{4.14}$$

$$C = \hbar AB = \frac{\hbar\omega}{2}. \tag{4.15}$$

With these, we may write

$$\begin{aligned}\hat{H} &= \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 \\ &= \left(\hat{q}\sqrt{\frac{m\omega^2}{2}} + \mathrm{i}\hat{p}\sqrt{\frac{1}{2m}}\right)^\dagger \left(\hat{q}\sqrt{\frac{m\omega^2}{2}} + \mathrm{i}\hat{p}\sqrt{\frac{1}{2m}}\right) + \frac{1}{2}\hbar\omega \\ &= \hbar\omega\left[\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right)^\dagger}_{=\hat{a}^\dagger}\underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}\right)}_{=:\hat{a}} + \frac{1}{2}\right] \\ &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right).\end{aligned} \tag{4.16}$$

Definition 4.5.1 *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

$$\begin{aligned}[\hat{a}, \hat{a}^\dagger] &= \frac{m\omega}{2\hbar}\left[\hat{q} + \frac{\mathrm{i}}{m\omega}\hat{p}, \hat{q} - \frac{\mathrm{i}}{m\omega}\hat{p}\right] \\ &= \frac{m\omega}{2\hbar}\left[\hat{q}, -\frac{\mathrm{i}}{m\omega}\hat{p}\right] + \left[\frac{\mathrm{i}}{m\omega}\hat{p}, \hat{q}\right] \\ &= \frac{\mathrm{i}}{2\hbar}\Big(- \underbrace{[\hat{q}, \hat{p}]}_{=\mathrm{i}\hbar} + \underbrace{[\hat{p}, \hat{q}]}_{=-\mathrm{i}\hbar} \Big) = 1.\end{aligned} \tag{4.17}$$

Some observations about the quantum harmonic oscillator:

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

$$\begin{aligned}\langle\hat{H}\rangle &= \langle\psi|\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|\psi\rangle \\ &= \frac{\hbar\omega}{2} + \langle\psi|\hbar\omega\hat{a}^\dagger\hat{a}|\psi\rangle \\ &= \hbar\omega\left(\frac{1}{2} + \|\hat{a}\,|\psi\rangle\,\|^2\right) \geq 0.\end{aligned} \tag{4.18}$$

   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,

$$\begin{aligned}\hat{H}\hat{a}\,|\psi\rangle &= \hbar\omega\Bigg(\underbrace{\hat{a}^\dagger\hat{a}}_{=\hat{a}\hat{a}^\dagger - 1} + \frac{1}{2}\Bigg)\hat{a}\,|\psi\rangle \\ &= \hat{a}\hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2} - 1\right)|\psi\rangle \\ &= \hat{a}\left(\hat{H} - \hbar\omega\right)|\psi\rangle \\ &= \hat{a}\left(\varepsilon - \hbar\omega\right)|\psi\rangle = (\varepsilon - \hbar\omega)\hat{a}\,|\psi\rangle\,.\end{aligned} \tag{4.19}$$

   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 $|0\rangle$:

$$\begin{aligned}\hat{H}|0\rangle &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)|0\rangle \\ &= \frac{\hbar\omega}{2}|0\rangle\,.\end{aligned} \tag{4.20}$$

Thus the spectrum of $\hat{H}$ is $\{\varepsilon_n\} = \left\{\hbar\omega\left(n+\frac{1}{2}\right)\right\}$, and the corresponding normalized eigenstates are simply written as $\{|n\rangle\}$. That is, $\hat{H}|n\rangle = \hbar\omega\left(n+\frac{1}{2}\right)|n\rangle$. From the spectrum we notice that the action of $\hat{a}^\dagger a$ on $|n\rangle$ is to count the number of times the energy has been raised from the ground state. For this reason,

$$\hat{N} = \hat{a}^\dagger\hat{a} = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2}, \tag{4.21}$$

$$\hat{N}|n\rangle = n|n\rangle \tag{4.22}$$

is called the *number operator*. It satisfies

$$[\hat{N},\hat{a}] = -\hat{a}, \qquad [\hat{N},\hat{a}^\dagger] = \hat{a}^\dagger. \tag{4.23}$$

If $|n\rangle$ is a normalized eigenstate of the Hamiltonian, then

$$\begin{aligned}||\hat{a}^\dagger|n\rangle|| &= \sqrt{\langle n|\hat{a}\hat{a}^\dagger|n\rangle} \\ &= \sqrt{\langle n|a^\dagger\hat{a}+1|n\rangle} \\ &= \sqrt{\langle n|\hat{N}+1|n\rangle} \\ &= \sqrt{(n+1)\langle n|n\rangle} \\ &= \sqrt{n+1}.\end{aligned} \tag{4.24}$$

Similarly,

$$||\hat{a}|n\rangle|| = \sqrt{n}. \tag{4.25}$$

Thus we conclude that even though $\hat{a}^\dagger|n\rangle$ and $\hat{a}|n\rangle$ (with $n \geq 1$) are still eigenvectors of the Hamitonian with eigenvalues $n+1$, and $n-1$, respectively, they are not normalized. Since we've labeled the normalized eigenstates as $\{|n\rangle\}$, we can write

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \tag{4.26}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle\,. \tag{4.27}$$

The second equation gives us an expression for any eigenstate in terms of the ground state:

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(\hat{a}^\dagger\right)^n|0\rangle \tag{4.28}$$

4.6 Heisenberg uncertainty relation

Above, we introduced an example of quantizing a system starting with the classical Lagrangian and Hamiltonian. A fundamental difference between the classical and quantum descriptions is *uncertainty*, or the notion that the values of conjugate observables cannot be known simultaneously to an arbitrary precision.

Definition 4.6.1 *The Heisenberg uncertainty relation is defined as*

$$\Delta q \Delta p \geq \frac{\hbar}{2}, \tag{4.29}$$

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

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

The Heisenberg uncertainty relation is obtained from the Robertson uncertainty relation by indentifying $\hat{A} = \hat{q}$ and $\hat{B} = \hat{p}$, from which it follows that $||[\hat{A}, \hat{B}]|| = ||[\hat{q}, \hat{p}]|| = |\mathrm{i}\hbar| = \hbar$.

Lecture 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,

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

Math on a diff.eq.

$\partial_x f(x) = \lambda f(x) \implies f(x) = f(0)\mathrm{e}^{\lambda x}$

The temporal evolution can thus 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 defined to be *unitary*.

Let $\{|\psi_n\rangle\} \in \mathcal{H}$ be an eigenbasis of the Hamiltonian $\hat{H}$, i.e., $\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle$, where $\{E_n\}_{n=0}^{\infty} \in \mathbb{R}$. 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

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

Consequently, the eigenstates and eigenenergies of the Hamiltonian yield the solution of the Schrödinger equation. Thus the time-dependent Schrödinger equation considered above, can also be cast into the following time-independent form:

Definition 5.2.2 *The time-independent Schrödinger equation is given*

by

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle\,, \tag{5.8}$$

where $\hat{H}$ is the Hamiltonian of the system and $\{E_n\}_n$ and $\{|\psi_n\rangle\}_n$ are its eigenenergies and eigenstates, respectively.

5.3 Case of temporally dependent Hamiltonian

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

$$\mathrm{i}\hbar\partial_t\,|\psi(t)\rangle = \hat{H}(t)\,|\psi(t)\rangle\,, \tag{5.9}$$

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

$$\hat{U}(t)\,|\psi(0)\rangle = |\psi(t)\rangle\,, \qquad \forall\,|\psi(t)\rangle \in \mathcal{H} \tag{5.10}$$

$$\Rightarrow \mathrm{i}\hbar\partial_t\left(\hat{U}(t)\,|\psi(0)\rangle\right) = \hat{H}(t)\left(\hat{U}(t)\,|\psi(0)\rangle\right) \tag{5.11}$$

$$\Rightarrow \mathrm{i}\hbar\partial_t\hat{U}(t) = \hat{H}(t)\hat{U}(t). \tag{5.12}$$

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

$$\left(\hat{U}_1\hat{U}_2\right)^\dagger = \hat{U}_2^\dagger\hat{U}_1^\dagger = \hat{U}_2^{-1}\hat{U}_1^{-1} = \left(\hat{U}_1\hat{U}_2\right)^{-1}. \tag{5.13}$$

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

$$|\psi'\rangle = \hat{U}\,|\psi\rangle \quad \text{and} \quad |\phi'\rangle = \hat{U}\,|\phi\rangle\,, \tag{5.14}$$

for which we have

$$\begin{aligned}\langle\psi|\phi\rangle &= \langle\psi|\hat{I}|\phi\rangle = \langle\psi|\hat{U}^{-1}\hat{U}|\phi\rangle \\ &= \langle\psi|\hat{U}^\dagger\hat{U}|\phi\rangle = \left(\hat{U}\,|\psi\rangle, \hat{U}\,|\phi\rangle\right) \\ &= \langle\psi'|\phi'\rangle\,.\end{aligned} \tag{5.15}$$

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 $\mathcal{H}_2 = \text{span}\{|\tilde{0}\rangle, |\tilde{1}\rangle\}$, 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

$$|\psi\rangle \in \mathcal{H}_2 \quad \text{and} \quad \| |\psi\rangle \| = 1. \tag{5.16}$$

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

3: Ground and excited

Thus,

$$\begin{aligned}\hat{H}_q &= \varepsilon_1 |g\rangle\langle g| + \varepsilon_2 |e\rangle\langle e| \\ &= \frac{\varepsilon}{2}\left(-|g\rangle\langle g| + |e\rangle\langle e|\right) + \frac{(\varepsilon_1+\varepsilon_2)}{2}|g\rangle\langle g| + \frac{(\varepsilon_1+\varepsilon_2)}{2}|e\rangle\langle e| \\ &= \frac{\varepsilon}{2}\left(-|g\rangle\langle g| + |e\rangle\langle e|\right) + \underbrace{\frac{\varepsilon_1+\varepsilon_2}{2}\hat{I}}\end{aligned} \tag{5.17}$$

We can disregard this since it just equally changes the phase of all $|\psi\rangle \in \mathcal{H}_2$

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

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

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

Thus,

$$\begin{aligned}\hat{H}_q &= -\frac{\varepsilon}{2}\hat{\sigma}_z, \qquad \hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \\ &\hat{=} \begin{bmatrix} -\frac{\varepsilon}{2} & 0 \\ 0 & +\frac{\varepsilon}{2} \end{bmatrix}.\end{aligned} \tag{5.18}$$

The temporal evolution is given by

$$\begin{aligned}|\psi(t)\rangle &= e^{-i\hat{H}_q t/\hbar}|\psi(0)\rangle, \qquad |\psi(0)\rangle = c_0|0\rangle + c_1|1\rangle \\ &= e^{+i\frac{\varepsilon}{2}\hat{\sigma}_z t/\hbar}|\psi(0)\rangle \\ &= e^{i\frac{\varepsilon}{2}t/\hbar}c_0|0\rangle + e^{-i\frac{\varepsilon}{2}t/\hbar}c_1|1\rangle.\end{aligned} \tag{5.19}$$

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

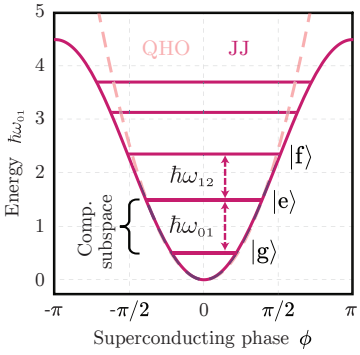

Figure 5.1: Non-linear harmonic oscillator with a Josephson junction (JJ). Notice that the gap $\hbar\omega_{01} \neq \hbar\omega_{12}$, i.e., the energy states are non-equidistant. Figure from Ref. [1].

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. It is useful to contrast a QHO to a qubit – QHO has an infinite number of states, separated by the same level spacing of $\hbar\omega$, while a qubit has only two states. Thus, a qubit is in some sense the most "anharmonic" quantum system possible. You can think of making a qubit from a QHO by pushing all the levels beyond the first excited state so high in energy that they cannot be occupied in practice.

5.7 Pauli operators

Definition 5.7.1 *The Pauli operators are*

$$\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \tag{5.20}$$
$$\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \tag{5.21}$$
$$\hat{\sigma}_y = -\mathrm{i}\,|0\rangle\langle 1| + \mathrm{i}\,|1\rangle\langle 0| \tag{5.22}$$

Properties

The Pauli operators have a number of interesting properties:

$$\hat{\sigma}_\alpha^2 = \hat{I} \qquad \forall \alpha \in \{\mathrm{x},\mathrm{y},\mathrm{z}\} \tag{5.23}$$
$$\hat{\sigma}_\alpha^\dagger = \hat{\sigma}_\alpha \qquad \forall \alpha \tag{5.24}$$
$$[\hat{\sigma}_i, \hat{\sigma}_j] = \sum_{k\in\{\mathrm{x},\mathrm{y},\mathrm{z}\}} 2\mathrm{i}\hat{\sigma}_k \varepsilon_{ijk}, \qquad \forall i,j \in \{\mathrm{x},\mathrm{y},\mathrm{z}\}, \tag{5.25}$$

where

$$\varepsilon_{ijk} = \begin{cases} +1 & \text{if } (i,j,k) \in \{(\mathrm{x},\mathrm{y},\mathrm{z}),(\mathrm{z},\mathrm{x},\mathrm{y}),(\mathrm{y},\mathrm{z},\mathrm{x})\}, \\ -1 & \text{if } (i,j,k) \in \{(\mathrm{y},\mathrm{x},\mathrm{z}),(\mathrm{z},\mathrm{y},\mathrm{x}),(\mathrm{x},\mathrm{z},\mathrm{y})\}, \\ 0 & \text{otherwise,} \end{cases} \tag{5.26}$$

is the Levi-Civita symbol.

Definition 5.7.2

$$\hat{\sigma}^- = |0\rangle\langle 1| \tag{5.27}$$
$$\hat{\sigma}^+ = (\hat{\sigma}^-)^\dagger = |1\rangle\langle 0|\,. \tag{5.28}$$

Exercise

Show that

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

where $\vec{a} \in \mathbb{R}^3$, $\|\vec{a}\| = 1$ and $\vec{a} \cdot \hat{\vec{\sigma}} = a_x\hat{\sigma}_x + a_y\hat{\sigma}_y + a_y\hat{\sigma}_z$.

5.8 Bloch sphere

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

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle, \tag{5.29}$$

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

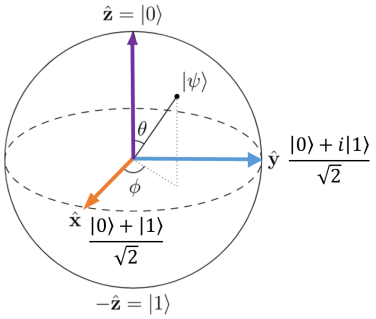

Figure 5.2: Bloch sphere representation [2].

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

$$\langle\psi|\hat{A}|\psi\rangle = \langle\psi|\hat{A}e^{-i\alpha}e^{i\alpha}|\psi\rangle = \langle\psi|e^{-i\alpha}\hat{A}e^{i\alpha}|\psi\rangle = \langle e^{i\alpha}\psi|\hat{A}e^{i\alpha}|\psi\rangle, \tag{5.30}$$

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

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

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

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

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 $\vec{H}_{\mathrm{ex}}(t) = \frac{\Omega}{2}\hat{\sigma}_x \sin(\omega t + \phi)$, 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

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

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

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

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

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

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:

- $\mathcal{H}_{2^n} = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)} \otimes \cdots \otimes \mathcal{H}_2^{(n)}$

- $|\psi\rangle = \sum_{k=0}^{2^n-1} c_k |k\rangle = c_0 |\underbrace{00\cdots0}_{n \text{ zeroes}}\rangle + c_1 |\underbrace{0\cdots01}_{n-1 \text{ zeroes}}\rangle + \cdots$, 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 $\hat{A}$.

Lecture 7

7.1 Intended learning outcomes

- Identify continuous bases for Hilbert spaces
- Apply the eigenstate of the position operator to obtain the wave function from the quantum state
- Identify the momentum operator in the position basis and apply it to obtain the Schrödinger equation in the position basis
- Apply creation and annihilation operators in the position basis to obtain the wave functions of the eigenstates of the harmonic oscillator

7.2 Continuous bases

If a quantum system has some continuous variable, it can be useful to express the state vectors in a continuous basis.

Let $\{|\psi_\alpha\rangle\}_{\alpha\in\mathbb{R}} \in \mathcal{H}$ be such that

$$\langle\psi_\alpha|\psi_{\alpha'}\rangle = \delta(\alpha - \alpha'), \tag{7.1}$$

where $\alpha, \alpha' \in \mathbb{R}$ and $\delta(x)$ is the Dirac delta function. Such a set of vectors is a *continuous basis* for $\mathcal{H}$.

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

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

$$\begin{aligned} |\psi\rangle &= \int c_\alpha\, |\psi_\alpha\rangle\, \mathrm{d}\alpha \\ &= \int \langle\psi_\alpha|\psi\rangle|\psi_\alpha\rangle\, \mathrm{d}\alpha \\ &= \int |\psi_\alpha\rangle\langle\psi_\alpha|\psi\rangle\, \mathrm{d}\alpha = \underbrace{\left(\int |\psi_\alpha\rangle\langle\psi_\alpha|\, \mathrm{d}\alpha\right)}_{\hat{I}} |\psi\rangle \end{aligned} \tag{7.2}$$

This is equivalent to the result of Eq. (2.4) in the continuous case.

Math on Dirac delta function

For a smooth function, i.e., $f \in C^\infty$, the Dirac delta is defined as the *generalized function* δ that satisfies

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

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.

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 $\langle \psi_\alpha | \psi \rangle \coloneqq \psi(\alpha)$, where $\psi(\alpha) : \mathbb{R} \to \mathbb{C}$ is generally referred to as the *wave function*.

Using the definition of the identity operator from Eq. (7.2) above, we observe that the inner product between any two vectors $|\phi\rangle$ and $|\chi\rangle$ of $\mathcal{H}$ is given in the continuous basis by

$$\begin{aligned} \langle \phi | \chi \rangle &= \langle \phi | \left(\int |\psi_\alpha\rangle \langle \psi_\alpha| \, \mathrm{d}\alpha \right) |\chi\rangle \\ &= \int \langle \phi | \psi_\alpha \rangle \langle \psi_\alpha | \chi \rangle \, \mathrm{d}\alpha \\ &= \int \phi^*(\alpha) \chi(\alpha) \mathrm{d}\alpha, \end{aligned} \tag{7.3}$$

where $\phi^*(\alpha) \coloneqq (\phi(\alpha))^*$.

The most common example of a continuous basis and the corresponding wave function is the *position basis*. Often, the state $|\psi\rangle$ describes some particle, such as an atom or electron. In this case, the eigenstate that corresponds to finding the particle at a position $x \in \mathbb{R}$ is written as just $|x\rangle$ (instead of $|\psi_x\rangle$).[2] The wave function is then a function of position: $\psi(x) \coloneqq \langle x | \psi \rangle$, and the probability density of finding the particle at x is $|\psi(x)|^2$.

2: Here we consider a particle lying on a one-dimensional line, but this treatment can be extended to three dimensions, where $x \in \mathbb{R}$ is replaced by $\vec{x} \in \mathbb{R}^3$.

Again using the trick of inserting the identity operator, we can find the position basis representation of a state $|\psi\rangle$ as an integral over the eigenstates of the position basis $|x\rangle$:

$$\begin{aligned} |\psi\rangle = \hat{I} |\psi\rangle &= \left(\int |x\rangle\langle x| \, \mathrm{d}x \right) |\psi\rangle \\ &= \int |x\rangle \langle x | \psi \rangle \, \mathrm{d}x \\ &= \int |x\rangle \underbrace{\psi(x)}_{\in \mathbb{C}} \, \mathrm{d}x \\ &= \int \psi(x) |x\rangle \, \mathrm{d}x. \end{aligned} \tag{7.4}$$

This is analogous to the discrete basis case, where we wrote $|\psi\rangle = \sum_k c_k |\phi_k\rangle$.

Note that wave functions cannot fully describe all quantum systems, only those where such continuous variables exist and are sufficient.

Definition 7.2.1 *In a continuous basis $\{|\psi\rangle_\alpha\}$, the measurement probability of the measurement outcome to reside in the interval $[\alpha, \alpha + d\alpha]$ is defined by*

$$dP(\alpha) = |\langle \psi_\alpha | \psi \rangle|^2 \, d\alpha. \tag{7.5}$$

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

$$\partial_{\hat{q}} f(\hat{q})\,|\psi\rangle = \left[f'(\hat{q}) + f(\hat{q})\partial_{\hat{q}}\right]|\psi\rangle\,, \tag{7.6}$$

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

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

$$\begin{aligned}
[\hat{q}, \hat{p}] &= \hat{q}\hat{p} - \hat{p}\hat{q} \\
&= \hat{q}\left(-\mathrm{i}\hbar\partial_{\hat{q}}\right) - \left(-\mathrm{i}\hbar\partial_{\hat{q}}\right)\hat{q} \\
&= -\mathrm{i}\hbar\hat{q}\partial_{\hat{q}} + \mathrm{i}\hbar\partial_{\hat{q}}\hat{q} \\
&= -\mathrm{i}\hbar\hat{q}\partial_{\hat{q}} + \mathrm{i}\hbar\underbrace{\left(\partial_{\hat{q}}\hat{q}\right)}_{=\hat{I}} + \mathrm{i}\hbar\hat{q}\partial_{\hat{q}} \\
&= \mathrm{i}\hbar.
\end{aligned} \tag{7.7}$$

Thus if follows that the representation of the canonical momentum operator in the coordinate basis is given by

$$\langle x'|\hat{p}|x\rangle = -\mathrm{i}\hbar\delta(x' - x)\partial_x. \tag{7.8}$$

7.4 Finding the eigenstates of energy for the quantum harmonic oscillator in the position representation

The algebraic solution of the quantum harmonic oscillator discussed in Chapter 4 is mathematically very elegant and convenient: it is simple to manipulate and has a simple solution. However, it is somewhat abstract and may call for additional analysis to relate the results to the physics of the system. Here, we derive the wave functions of the eigenstates, i.e. their representation in real physical space.

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

$$
\begin{aligned}
0 &= \langle x'|\hat{a}|0\rangle \qquad (7.9)\\
&= \langle x'| \underbrace{\sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{\mathrm{i}}{m\omega}(-\mathrm{i}\hbar\partial_{\hat{x}})\right)}_{=\hat{a}} \underbrace{\left(\int \mathrm{d}\tilde{x}\,|\tilde{x}\rangle\langle\tilde{x}|\right)}_{=\hat{I}} |0\rangle \\
&= \sqrt{\frac{m\omega}{2\hbar}} \int \mathrm{d}\tilde{x}\, \underbrace{\langle x'|\tilde{x}\rangle}_{\delta(\tilde{x}-x')} \left(\tilde{x} + \frac{\hbar}{m\omega}\partial_{\tilde{x}}\right) \underbrace{\psi_0(\tilde{x})}_{=:\langle\tilde{x}|0\rangle}
\end{aligned}
$$

$$
\Rightarrow \left(x + \frac{\hbar}{m\omega}\partial_x\right)\psi_0(x) = 0 \qquad (7.10)
$$

$$
\Rightarrow \psi_0(x) = C\exp\left(-\frac{x^2 m\omega}{2\hbar}\right), \qquad (7.11)
$$

where $C = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}$ is a normalization coefficient.Using definitions 4.5.1 and 4.28, we can then write

$$
\psi_n(x) = \frac{1}{\sqrt{n!}}\left[\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{\hbar}{m\omega}\frac{\partial}{\partial x}\right)\right]^n \psi_0(x). \qquad (7.12)
$$

For instance, the first excited state ψ_1 assumes the form

$$
\psi_1(x) = -C\sqrt{\frac{m\omega}{2\hbar}}\, x \exp\left(-\frac{x^2 m\omega}{2\hbar}\right). \qquad (7.13)
$$

The real-valued amplitude of the ground-state wave function and those of the five first excited states are depicted in Fig. 7.1. The probability densities, i.e., the absolute value squared of the wave function, are illustrated in Fig. 7.2.

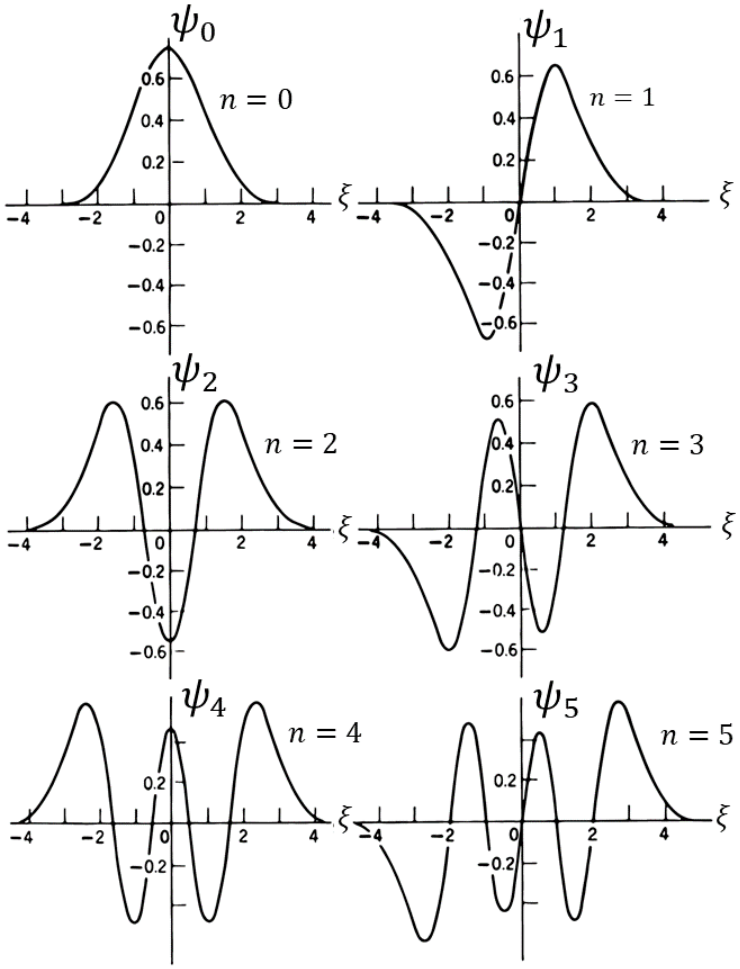

Figure 7.1: Real-valued wave functions of the quantum harmonic oscillator as functions of position $\xi = x$.

7.5 Schrödinger equation in the position basis

For a system described by continuous generalized coordinates $\{q_k\}_k$ and momenta $\{p_k\}_k$, the derivation of the Schrödinger equation

$$i\hbar\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle , \tag{7.14}$$

according to the above-described method yields the classical Hamiltonian function $H(\{q_k\}, \{p_k\})$ which yield the Hamiltonian operator $\hat{H} = H(\{\hat{q}_k\}, \{\hat{p}_k\})$ according to the operator substitution.

To obtain the Schrödinger equation in the position basis, we define the wave function $\psi(\{q_k\}, t) = \langle\{q_k\}|\psi(t)\rangle$ and take the inner product of the Schrödinger equation with the eigenstate of the

position basis as

$$
\begin{aligned}
&\mathrm{i}\hbar\partial_t \langle\{q_k\}|\psi(t)\rangle = \langle\{q_k\}|\hat{H}|\psi(t)\rangle \\
&= \mathrm{i}\hbar\partial_t\psi(\{q_k\},t) = \langle\{q_k\}|\hat{H}\int \mathrm{d}\{\tilde{q}_k\}\,|\{\tilde{q}_k\}\rangle\langle\{\tilde{q}_k\}|\,|\psi(t)\rangle \\
&\qquad = \int \mathrm{d}\{\tilde{q}_k\}\,\langle\{q_k\}|\hat{H}|\{\tilde{q}_k\}\rangle\,\psi(\{\tilde{q}_k\},t) \\
&\qquad = \int \mathrm{d}\{\tilde{q}_k\}\delta(\{q_k-\tilde{q}_k\})H(\{q_k\},\{-\mathrm{i}\hbar\partial_{q_k}\})\psi(\{\tilde{q}_k\},t) \\
&\qquad = H(\{q_k\},\{-\mathrm{i}\hbar\partial_{q_k}\})\psi(\{q_k\},t), \qquad (7.15)
\end{aligned}
$$

where H is the classical Hamiltonian function and $\delta(\{q_k-\tilde{q}_k\})$ is a multidimensional Dirac delta function. Thus we have reduced the original Schrödinger equation into a partial differential equation. Note that here we have assumed that there are only continuous generalized coordinates. In the case of spin degrees of freedom that are discrete, one needs to consider them to promote the multivariable wave function into a vector referred to as a *spinor*.

7.6 Schrödinger equation of the quantum harmonic oscillator in the position basis

In the case of the one-dimensional harmonic oscillator, obtained as a special case of the above general framework, we have $H(p,q) = p^2/(2m) + m\omega^2 q^2/2$, which yields the position representation of the Schrödinger equation as

$$
\mathrm{i}\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + \frac{m\omega^2}{2}x^2\psi(x,t). \qquad (7.16)
$$

The wave functions of the eigenstates in Eq. (7.12) thus obey the time-independent Schrödinger equation

$$
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_n(x) + \frac{m\omega^2}{2}x^2\psi_n(x) = E_n\psi_n(x), \qquad (7.17)
$$

where the eigenenergy $E_n = \hbar\omega(n+1/2)$ we derived below Eq. (4.20). Note that the spectrum of an operator is independent of the basis used to solve the spectrum.

Appendix A.1 describes the traditional way of solving the eigenstates and the spectrum of the quantum harmonic oscillator from the second-order partial differential equation (7.16). For the sake of time, we do not treat this method in detail. Instead, we merely note that the this method provides us another expression for the

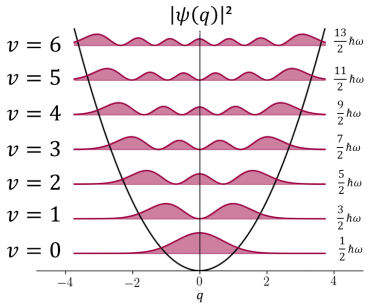

Figure 7.2: Probability density of finding a particle in a quadratic potential well at any given point for the seven lowest-energy eigenstates of the Hamiltonian.

eigenstates in Eq. (7.12) as

$$\psi_n(x) = 2^{-\frac{n}{2}}(n!)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad (7.18)$$

where $\{H_n(\cdot)\}_n$ are special functions referred to as Hermite polynomials. The properties and the exact forms of these functions are tabulated in typical mathematics reference books and in Wikipedia.

Lecture 8 | 8

This lecture describes a quantum particle in various external potentials, including cases where the particle is either trapped or it can propagate and scatter in real space. Such systems are naturally treated in the position basis by explicitly solving the corresponding Schrödinger equation with proper boundary conditions. We begin with the case of a free particle, highlighting the choice of different bases (position or momentum here). We then discuss the influence of external potentials and the differences between pointlike classical particles and quantum particles.

8.1 Intended learning outcomes

- Apply the position and momentum bases to represent the position and momentum operators in them
- Apply the time-dependent Schrödinger equation on the free particle to arrive at plane wave solutions
- Differentiate between a particle in a box and a particle in a finite potential well

8.2 Eigenstates of the position and momentum operators and their connection to the free Particle

Consider in one dimension, a free particle that does not experience any external potentials, i.e., $V(q) = 0$ in the classical Laplace function. Thus, the Schödinger equation has only the kinetic-energy term consisting of the momentum operator. To describe such a particle, we consequently examine the eigenstates of the position and momentum operators as

$$\hat{x}|x\rangle = x|x\rangle; \qquad \hat{p}|p\rangle = p|p\rangle\,. \tag{8.1}$$

Owing to the fact that the position and momentum operators are Hermitian, the corresponding bra vectors obey

$$\langle x|\hat{x} = \langle x|x; \qquad \langle p|\hat{p} = \langle p|p. \tag{8.2}$$

We choose the normalization of these continuous bases as in Sec. 7.2:

$$\langle x'|x\rangle = \delta(x'-x); \qquad \langle p'|p\rangle = \delta(p'-p), \tag{8.3}$$

and note that each of these sets of operators form complete orthonormal set. The corresponding identity operator can be inserted between any states when necessary (see Sec. 7.2 for derivation):

$$\int \mathrm{d}x|x\rangle\langle x| = \hat{I}; \qquad \int \mathrm{d}p|p\rangle\langle p| = \hat{I}. \tag{8.4}$$

As derived in Sec. 7.3, the ***momentum operator*** *is represented in the position basis* as

$$\langle x'|\hat{p}|x\rangle = -\mathrm{i}\hbar\,\delta(x'-x)\partial_x. \tag{8.5}$$

This equation, stemming from the canonical commutation relation, connects the position and momentum bases together.

In a similar manner, we can derive the ***position operator*** *in the momentum basis* as

$$\langle p'|\hat{x}|p\rangle = +\mathrm{i}\hbar\,\delta(p'-p)\partial_p. \tag{8.6}$$

Next, we solve the *eigenstates of the momentum operator in the position basis* $\psi_p(x) = \langle x|p\rangle$ by first noting that

$$\langle x|\hat{p}|p\rangle = p\langle x|p\rangle. \tag{8.7}$$

On the other hand, we have

$$\langle x|\hat{p}|p\rangle = \int \mathrm{d}x'\langle x|\hat{p}|x'\rangle\langle x'|p\rangle = \int \mathrm{d}x' - \mathrm{i}\hbar\,\delta(x-x')\partial_{x'}\langle x'|p\rangle \tag{8.8}$$

$$= -\mathrm{i}\hbar\partial_x\langle x|p\rangle. \tag{8.9}$$

Thus, by equation the two above identities, we arrive at the differential equation

$$-\mathrm{i}\hbar\partial_x\langle x|p\rangle = p\langle x|p\rangle. \tag{8.10}$$

The solution to this equation is referred to as a simple plane wave

$$\langle x|p\rangle = \sqrt{\frac{1}{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar}, \tag{8.11}$$

where the normalization coefficient can be solved using Eq. (8.3) and writing $\langle x'|x\rangle = \langle x'|\left(\int \mathrm{d}p|p\rangle\langle p|\right)|x\rangle = \int \mathrm{d}p\,\langle x'|p\rangle\,\langle p|x\rangle = \delta(x'-x)$.[1]

1: Note that the Dirac delta fucntion has the properties $\delta(x) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\mathrm{e}^{\mathrm{i}xp/\hbar}\mathrm{d}p$ and $\delta(ax) = |a|^{-1}\delta(x), \forall a \neq 0$.

Note that the normalized *position eigenstate in the momentum basis* can be obtained from

$$\langle p|x\rangle = \langle x|p\rangle^* = \sqrt{\frac{1}{2\pi\hbar}} e^{-ipx/\hbar}, \tag{8.12}$$

and the normalized *position eigenstate in the position basis* is given by the normalizaiton condition in Eq. (8.3) as

$$\langle x'|x\rangle = \delta(x - x'). \tag{8.13}$$

Note that the dimension of the wave function above $\psi_p(x) = \langle x|p\rangle$ is not $1/\sqrt{\text{length}}$ because in addition to $\{|x\rangle\}$, also $\{|p\rangle\}$ is a continuous basis and hence bears dimension according to Eqs. (8.3) and (8.4).

Let us come back to our case of the free particle, the Hamiltonian operator of which is $\hat{H} = \hat{p}^2/(2m)$. This Hamiltonian co-indices with that of the quantum harmonic oscillator with zero potential. In the position basis, the time-independent Schrödinger equation reads

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle\,; \tag{8.14}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\psi_p(x)}{\partial x^2} = E_p\psi_p(x). \tag{8.15}$$

The above-derived eigensates of the momentum operator provide also the solution of this differential equation with $E_p = p^2/(2m)$. Note that each finite energy is doubly degenerate since $E_{-p} = E_p$.

8.3 Temporal dependence of plane waves

Let us look at the temporal dependence of the plane waves in the position basis. The time-dependent Schrödinger equation $i\hbar\partial_t\Psi = \hat{H}\Psi$ for a free particle can be represented as

$$i\hbar\partial_t\Psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\Psi(x,t). \tag{8.16}$$

We look for separable solutions of the form

$$\Psi(x,t) = f(t)\psi(x). \tag{8.17}$$

This gives

$$\frac{i\hbar}{f(t)}\frac{\partial f(t)}{\partial t} = -\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}. \tag{8.18}$$

Since there is no temporal dependence on the right side of the equation and no spatial dependence on the left side of the equation,

both sides must be equal to constant, let us say E_p that has the units of energy. Thus, we have

$$f(t) = \mathrm{e}^{-\mathrm{i}E_p t/\hbar}. \tag{8.19}$$

Using the plane wave from Eq. (8.11), the temporal evolution of the plane wave in the position basis is thus given by

$$\Psi(x,t) = \mathrm{e}^{-\mathrm{i}E_p t/\hbar}\langle x|p\rangle = \sqrt{\frac{1}{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}E_p t/\hbar}\mathrm{e}^{\mathrm{i}px/\hbar}, \tag{8.20}$$

where the energy dispersion relation for plane waves is $E_p = p^2/(2m)$. These are called *stationary states* because

$$\partial_t \left|\Psi(x,t)\right|^2 = 0. \tag{8.21}$$

For a general state that is a superposition of plane waves with coefficients c_p at time $t = 0$,

$$\Psi(x,0) = \sum_p c_p \mathrm{e}^{\mathrm{i}px/\hbar}, \tag{8.22}$$

the general solution of the time-dependent wave equation is simply

$$\Psi(x,t) = \sum_p c_p \mathrm{e}^{-\mathrm{i}E_p t/\hbar}\mathrm{e}^{\mathrm{i}px/\hbar} = \sum_p c_p \mathrm{e}^{\mathrm{i}(x - tE_p/p)p/\hbar}, \tag{8.23}$$

where the last equality shows that each component p corresponds to a wave that is traveling with velocity $E_p/p = p/(2m)$. Note that p can be positive or negative.

An important generalization of this result is that since the eigenstates of energy form a basis of the Hilbert space, we can use the wave functions of the eigenstates $\{\psi_p(x)\}_p$ to expand other wave functions. Note that here p does not need to be the momentum but can be any variable that indexes the states in a well-defined manner. In general, if it holds that for a wave function

$$\Psi(x,0) = \sum_p c_p \psi_p(x) \tag{8.24}$$

the time dependence of the wave function is given by

$$\Psi(x,t) = \sum_p c_p \mathrm{e}^{-\mathrm{i}E_p t/\hbar}\psi_p(x). \tag{8.25}$$

Equivalently, for a continuous energy spectrum, where the coefficients c_p correspond to a continuous function $c(p)$ of energy, we

have

$$\Psi(x,0) = \int c(p)\psi_p(x)\mathrm{d}p, \tag{8.26}$$

and the temporal evolution is given by

$$\Psi(x,t) = \int c(p)\psi_p(x)\mathrm{e}^{-\mathrm{i}E_p t/\hbar}\mathrm{d}p. \tag{8.27}$$

These results are equivalent to Eq. (5.7) expressed in the position basis.

8.4 Periodic boundary conditions

There is a mathematical subtlety associated with plane waves because owing to the absence of a binding potential, they extent to an infinite domain and are not normalizable. Curiously, this apparent dilemma is absent if we consider a length $L > 0$ and periodic boundary conditions $\psi_p(x) = \psi_p(x+L)$, but no external potential $V(x)$. Such a case with $L = 2\pi l$ naturally arises for example in the case of the pendulum of length l in no gravitational potential, i.e., $g = 0$ (see Fig. 4.1 but consider that there is no ceiling, i.e., the angle θ extends from 0 to 2π). The solution of such a Schrödinger equation is that of a free particle, but the momentum is quantized and can be written in terms of the wave number k_n as

$$p_n = \hbar k_n = \frac{2\hbar\pi n}{L}, \qquad n \in \mathbb{Z}. \tag{8.28}$$

The completeness relations read

$$\int_0^L \mathrm{d}x|x\rangle\langle x| = 1; \quad \sum_{n=-\infty}^{\infty} |p_n\rangle\langle p_n| = 1. \tag{8.29}$$

The eigenstate of the momentum operattor in the position basis is thus given by

$$\psi_{p_n}(x) = \langle x|p_n\rangle = \langle p_n|x\rangle^* = \frac{1}{\sqrt{L}}\mathrm{e}^{\mathrm{i}p_n x/\hbar} = \frac{1}{\sqrt{L}}\mathrm{e}^{\mathrm{i}k_n x}, \tag{8.30}$$

where $k_n = p_n/\hbar = 2\pi n/L$ is referred to as the *wave number*. Here the eigenstates are normalizable, and hence the normalization coefficient $1/\sqrt{L}$ in the above equation can be simply obtained from $||\,|p_n\rangle\,||^2 = 1 = \int_0^L |\psi_{p_n}(x)|^2\mathrm{d}x$.

8.5 Particle in an infinite potential well

The simplest case is that of a particle confined between two infinite walls as in Fig. 8.1, where

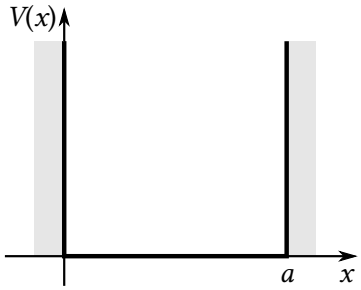

Figure 8.1: Infinite potential well.

$$V(x) = \begin{cases} 0, & \text{if } 0 \le x \le a; \\ \infty, & \text{otherwise.} \end{cases} \tag{8.31}$$

Since there is no potential in the well, the solution of the time-independent Schrödinger equation is there that of a free particle:

$$\psi''(x) = -k^2\psi(x); \qquad k = \frac{\sqrt{2mE}}{\hbar}. \tag{8.32}$$

Curiously, this equation corresponds to the equation of motion for a classical harmonic oscillator, the solutions of which are simple sine and cosine waves

$$\psi(x) = A\sin(kx) + B\cos(kx), \tag{8.33}$$

where $A, B \in \mathbb{C}$ are constants to be determined from the boudanry conditions and normalization.

Because the potential is infinite outside the well, the wave function must vanish there. Otherwise the energy would diverge, and we consider here only finite, but yet unknown, energies E. Thus $B = 0$ and hence

$$\psi(x) = A\sin(kx); \qquad ka = 0, \pm\pi, \pm 2\pi, \cdots, \tag{8.34}$$

where the quantization of the wave number $k_n = n\pi/a$ for $n \in \mathbb{Z}$ and the energy

$$E_n = \frac{\hbar^2 k_n^2}{2m}, \tag{8.35}$$

arises from the requirement $\sin(ka) = 0$. Normalization of the wave function gives

$$A = \sqrt{\frac{2}{a}}, \tag{8.36}$$

resulting in

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), \qquad n \in \mathbb{Z}_+, \tag{8.37}$$

where we have taken only the positive values of n since $n = 0$ leads to a zero wave function that is not normalizeable and every

negative n yields an indentical wave function to that of a posivite n apart from a phase factor. Eq. (8.37) is illustrated for the first three values of n in Fig. 8.2.

The stationary states of the time-dependent Schrödinger equation can be obtained from the general result $|\psi_n(t)\rangle = \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\,|\psi_n(0)\rangle$ [see Eq. (5.7)] and expressed as

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\mathrm{e}^{-\mathrm{i}E_n t/\hbar}. \tag{8.38}$$

The most general solution to the time-dependent Schrödinger equation can be written as

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\mathrm{e}^{-\mathrm{i}E_n t/\hbar}, \tag{8.39}$$

where the expansion coefficients $\{c_n\}$ are determined by the initial state $\Psi(x,0)$ through $c_n = \langle\psi_n|\Psi(0)\rangle = \int_{-\infty}^{\infty}\psi_n^*(x)\Psi(x,0)\,\mathrm{d}x$.

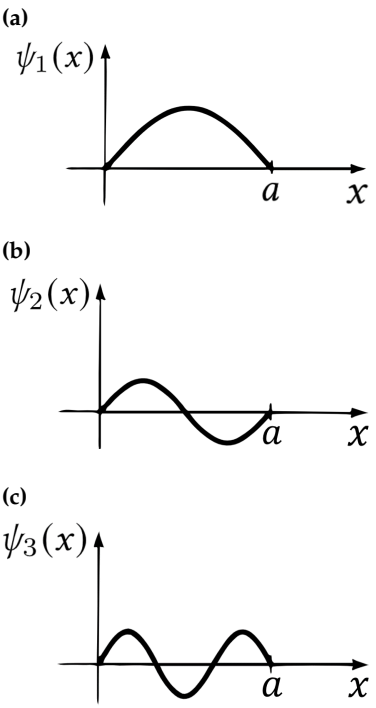

Figure 8.2: Wave function Eq. (8.37) for the modes (a) $n = 1$, (b) $n = 2$. (c) $n = 3$.

8.6 Particle in a square-well potential

Another simple but less trivial example is that of a quantum particle in a one-dimensional *square-well potential* (Fig. 8.3):

$$V(x) = \begin{cases} \infty, & \text{if } -\infty \le x \le 0; \\ -V_0, & \text{if } 0 \le x \le a, \\ 0, & \text{if } a \le x \le \infty. \end{cases} \tag{8.40}$$

We note this example here since it turns out in the detailed analysis[2] carried out in Appendix A.2 that there are two types of eigenstates of the Hamiltonian: *bound* states that are localized in the potential well with negative energy in reference to the zero level of the

2: You may read the appendix if you wish, but it will not be discussed in detail in during the lectures.

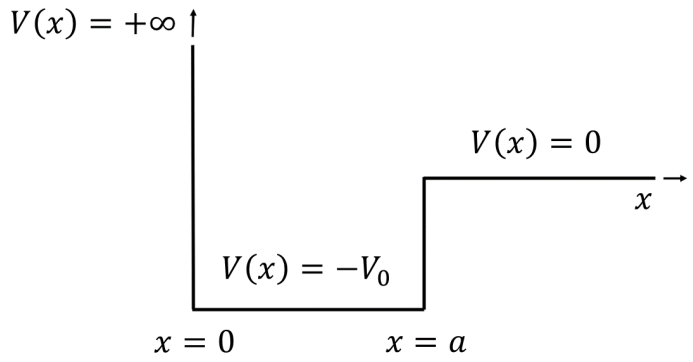

Figure 8.3: Square-well potential.

potential and *unbound* states that extent to infinity with positive energy. See Fig. 8.4 for an example of a wave function of an unbound state.

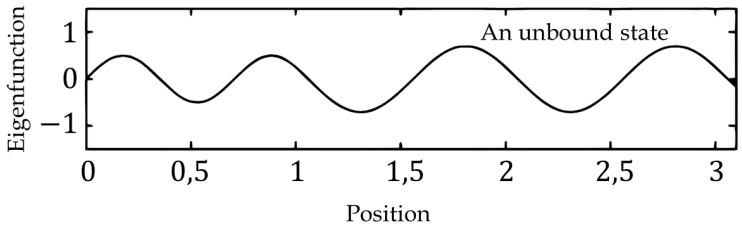

Figure 8.4: Example wave function corresponding to an eigenstate of energy of an unbound state. The position is in units of the width of the square-well potential a.

Lecture 9

This lecture deepens the quantum description of the physical phenomena associated with the motion of a point-like particle in external potentials. In the quantum description, the influence of an external potential on a particle is fundamentally different way from that of the classical description. In particular, a quantum particle can scatter back from a finite potential barrier such that only part of its wave function propagates across it. The second important quantum property is that of tunneling—a quantum particle has a finite probability to penetrate through a barrier of higher energy than the kinetic energy of the particle. Such tunneling is forbidden in the purely classical description of the motion, but yet used in quantum technology around the world.

9.1 Intended learning outcomes

- Identify the transmission and reflection proabilities
- Differentiate the quantum features in scattering from the classical case
- Identify the scattering matrix

9.2 Finite potential barrier: Scattering and tunneling

The first nontrivial case we consider for tunneling and scattering is that of a finite square-shaped potential barrier, see Fig. 9.1, given by

$$V(x) = \begin{cases} 0, & \text{if } -\infty < x < 0; \\ V_{\mathrm{B}}, & \text{if } 0 < x < a; \\ 0, & \text{if } a < x < +\infty. \end{cases} \tag{9.1}$$

To obtain the full time-dependent solution of this problem, we would need to write the wave function in the form of Eq. (8.27). However, for now we consider the eigensolutions of the Schrödinger equation as in Lecture 8 and focus on the properties of the waves traveling in this potential.

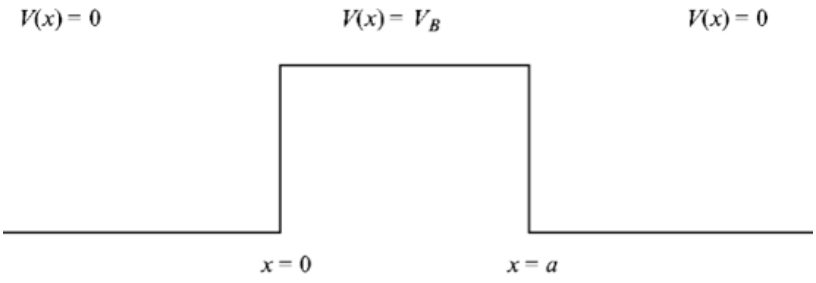

Figure 9.1: Finite square-shaped one-dimensional potential barrier.

First, on the left side of the barrier, we have

$$\psi_E''(x) = -k^2\psi_E(x); \qquad E = \frac{\hbar^2 k^2}{2m}, \qquad \text{for } x < 0, \tag{9.2}$$

with the solution

$$\psi_E(x) = A_{\mathrm{I}}\mathrm{e}^{\mathrm{i}kx} + A_{\mathrm{R}}\mathrm{e}^{-\mathrm{i}kx}, \qquad \text{for } x < 0, \tag{9.3}$$

where the wave number $k > 0$ and the intensity of the *incident* wave is $|A_{\mathrm{I}}|^2$ and that of the *reflected* wave $|A_{\mathrm{R}}|^2$. By computing $\langle\hat{p}\rangle$, one may observe that the momentum is positive for the incident wave (moving to the right) and negative for the reflected wave (moving to the left). The full quantum state is a linear superposition of these two individual states.

If the energy of the incoming particle is greater than that of the barrier $E > V_{\mathrm{B}}$, a case in which classically crossing the barrier is allowed, we have

$$\psi_E''(x) = -k_{\mathrm{B}}^2\psi_E(x); \qquad E = \frac{\hbar^2 k_{\mathrm{B}}^2}{2m} + V_{\mathrm{B}}, \qquad \text{for } a < x < 0, \tag{9.4}$$

with the general solution given by

$$\psi_E(x) = A\mathrm{e}^{\mathrm{i}k_{\mathrm{B}}x} + A'\mathrm{e}^{-\mathrm{i}k_{\mathrm{B}}x}, \qquad \text{for } a < x < 0, \tag{9.5}$$

where $k_{\mathrm{B}} > 0$.

For $E < V_{\mathrm{B}}$, the region is classically forbidden, but the schrödinger equation yields

$$\psi_E''(x) = \beta^2\psi_E(x); \qquad E = -\frac{\hbar^2\beta^2}{2m} + V_{\mathrm{B}}, \qquad \text{for } a < x < 0, \tag{9.6}$$

and the general solution becomes a decaying exponential

$$\psi_E(x) = B\mathrm{e}^{-\beta x} + B'\mathrm{e}^{\beta x}, \qquad \text{for } a < x < 0, \tag{9.7}$$

where $\beta > 0$.

On the right side of the barrier, we have

$$\psi_E(x) = A_{\mathrm{T}}\mathrm{e}^{\mathrm{i}kx}; \qquad k = \frac{\sqrt{2Em}}{\hbar}, \qquad \text{for } x > 0, \tag{9.8}$$

where $k > 0$ and the left-moving part of the wave function vanishes since we assume that there is only one in-coming wave, that from the left, and there are no scattering centers on the right side of the barrier that could scatter back the transmitted wave.

Instead of trying to solve for all the different coefficients, the physically interesting quantities here are the ratios of the reflected and transmitted intensities

$$R = \frac{|A_{\mathrm{R}}|^2}{|A_{\mathrm{I}}|^2} \quad \text{and} \quad T = \frac{|A_{\mathrm{T}}|^2}{|A_{\mathrm{I}}|^2}. \tag{9.9}$$

These are referred to as reflection and transmission probabilities, for which we have

$$R + T = 1, \tag{9.10}$$

owing to the unitarity of the temporal evolution in quanutm meachanics.

We focus here on a particle with energy below the barrier:

$$\psi_E(x) = \begin{cases} A_{\mathrm{I}}\mathrm{e}^{+\mathrm{i}kx} + A_{\mathrm{R}}\mathrm{e}^{-\mathrm{i}kx}, & \text{if } -\infty < x < 0; \\ B\mathrm{e}^{-\beta x} + B'\mathrm{e}^{+\beta x}, & \text{if } 0 < x < a; \\ A_{\mathrm{T}}\mathrm{e}^{+\mathrm{i}kx}, & \text{if } a < x < +\infty. \end{cases} \tag{9.11}$$

Continuity of ψ_E and ψ_E' at $x = 0$ and a gives

$$A_{\mathrm{I}} + A_{\mathrm{R}} = B + B' \quad \text{and} \quad \mathrm{i}kA_{\mathrm{I}} - \mathrm{i}kA_{\mathrm{R}} = -\beta B + \beta B'; \tag{9.12}$$

$$B\mathrm{e}^{-\beta a} + B'\mathrm{e}^{+\beta a} = A_{\mathrm{T}}\mathrm{e}^{\mathrm{i}ka} \quad \text{and} \quad -\beta B\mathrm{e}^{-\beta a} + \beta B'\mathrm{e}^{+\beta a} = \mathrm{i}kA_{\mathrm{T}}\mathrm{e}^{\mathrm{i}ka}, \tag{9.13}$$

from which we obtain the amplitudes as a function of B

$$2\mathrm{i}kA_{\mathrm{I}} = -(\beta - \mathrm{i}k)\,B + (\beta + \mathrm{i}k)\,B'; \tag{9.14}$$

$$A_{\mathrm{T}}\mathrm{e}^{\mathrm{i}ka} = \frac{2\beta}{\beta - \mathrm{i}k}B\mathrm{e}^{-\beta a} \quad \text{and} \quad B' = B\mathrm{e}^{-2\beta a}\frac{\beta + \mathrm{i}k}{\beta - \mathrm{i}k}. \tag{9.15}$$

In the limit of a wide barrier where $\mathrm{e}^{-2\beta a} \ll 1$ we can approximate that $B' \ll B$, *i.e.*, $2\mathrm{i}kA_{\mathrm{I}} \approx -(\beta - \mathrm{i}k)\,B$, which yields

$$A_{\mathrm{T}}\mathrm{e}^{\mathrm{i}ka} \approx -\frac{4\mathrm{i}k\beta\mathrm{e}^{-\beta a}}{(\beta - \mathrm{i}k)^2}A_{\mathrm{I}}, \tag{9.16}$$

and

$$T \approx \frac{16k^2\beta^2}{\left(\beta^2 + k^2\right)^2} e^{-2\beta a}. \tag{9.17}$$

Using the definitions

$$k = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad \beta = \frac{\sqrt{2m\left(V_B - E\right)}}{\hbar}, \tag{9.18}$$

this can be expressed as

$$T \approx \frac{16E\left(V_B - E\right)}{V_B^2} e^{-2\beta a}, \quad \text{for } E < V_B. \tag{9.19}$$

This is an important result in quantum mechanics, called the (quantum-mechanical) *tunneling probability*. Its main message is that the tunneling probability (rate) below the barrier energy decays proportional to the exponential of the square root of the mass times the energy difference between the barrier and the system energy. This conclusion actually holds more generally and can be applied to many different cases with more complicated barriers.

9.3 Delta-Function Potential Well

The last case we consider here is that of a (non-analytic) delta-function potential well at $x = 0$, i.e., the following potential function:

$$V(x) = -\alpha\delta(x), \tag{9.20}$$

where $\delta(x)$ is the Dirac delta function

$$\delta(x) = \begin{cases} 0, & \text{if } x \neq 0; \\ \infty, & \text{if } x = 0, \end{cases} \quad \text{with} \quad \int_{\infty}^{\infty} \delta(x)\mathrm{d}x = 1, \tag{9.21}$$

as previously discussed in Section 7.2, and the scale factor $\alpha > 0$ is referred to as the strength or depth of the potential well since

$$\int_{-\infty}^{\infty} V(x)\mathrm{d}x = -\alpha. \tag{9.22}$$

This potential is sketched in Fig. 9.2, although note that it is difficult to draw a picture that meaningfully distinguishes $-\delta(x)$ and $-\alpha\delta(x)$.

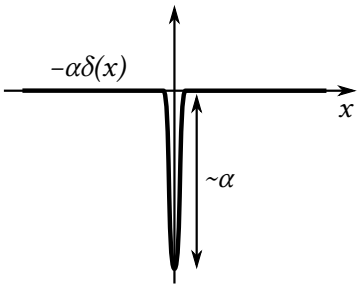

Figure 9.2: An approximation of the delta-function potential well with depth α.

With this potential, the eigenstates of energy in the position basis

obey

$$-\frac{\hbar^2}{2m}\psi''(x) - \alpha\delta(x)\psi(x) = E\psi(x). \tag{9.23}$$

The delta-function potential well supports both *bound* ($E < 0$) and *unbound*, or *scattering*, ($E > 0$) states. First, consider bound states with $x < 0$, where the Schrödinger equation reduces to

$$\psi''(x) = \kappa^2\psi(x); \qquad \kappa = \frac{\sqrt{-2mE}}{\hbar} > 0. \tag{9.24}$$

This has the decaying solution

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} = Be^{\kappa x}, \tag{9.25}$$

where $A = 0$ to ensure that $\lim_{x\to-\infty}\psi(x) = 0$.

Correspondingly, in the other half of the plane for positive x, the solution is

$$\psi(x) = Fe^{-\kappa x}. \tag{9.26}$$

From the previous examples, we have learned that the wave functions should satisfy the following conditions:

1. $\psi(x)$ is always continuous
2. $\frac{d\psi}{dx}$ is continuous except at the divergence points of the delta function

The first boundary condition is satisfied with $F = B$, see Fig. 9.3

$$\psi(x) = \begin{cases} Be^{\kappa x}, & \text{if } x \le 0; \\ Be^{-\kappa x}, & \text{if } x \ge 0. \end{cases} \tag{9.27}$$

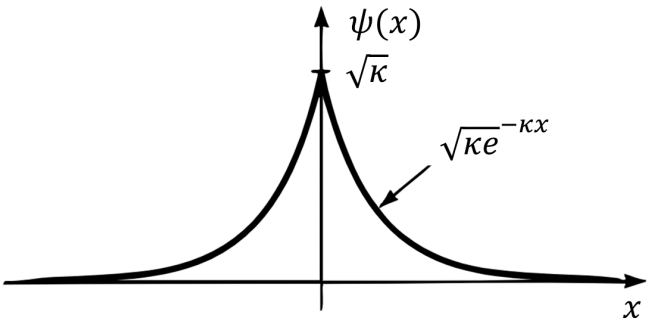

Figure 9.3: Bound state wave function for $E < 0$

The curiosity here is that the delta function potential does not enter the result as is. To examine this, we must study at the derivative at $x = 0$:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2\psi}{dx^2}dx + \int_{-\epsilon}^{\epsilon}V(x)\psi(x)dx = E\int_{-\epsilon}^{\epsilon}\psi(x)dx. \tag{9.28}$$

The left side yields a jump in the derivative as

$$\Delta\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = \frac{2m}{\hbar^2}\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} V(x)\psi(x)\mathrm{d}x, \tag{9.29}$$

and due to the delta function

$$\Delta\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}B. \tag{9.30}$$

Here

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \begin{cases} -B\kappa \mathrm{e}^{-\kappa x}, & \text{for } x>0, \text{ so } \frac{\mathrm{d}\psi}{\mathrm{d}x}\big|_{+} = -B\kappa; \\ +B\kappa \mathrm{e}^{+\kappa x}, & \text{for } x<0, \text{ so } \frac{\mathrm{d}\psi}{\mathrm{d}x}\big|_{-} = +B\kappa, \end{cases} \tag{9.31}$$

and thus $\Delta\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right) = -2B\kappa = -2m\alpha B/\hbar^2$, and hence the energy of the bound state is fixed to

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}. \tag{9.32}$$

Normalization gives

$$\int_{-\infty}^{\infty}|\psi(x)|^2\,\mathrm{d}x = 2|B|^2\int_0^{\infty}\mathrm{e}^{-2\kappa x}\mathrm{d}x = \frac{|B|^2}{\kappa} = 1. \tag{9.33}$$

Thus the main result is that the delta-function potential can support *one and only one bound state* which is given by

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\mathrm{e}^{-m\alpha|x|/\hbar^2} \quad \text{and} \quad E = -\frac{m\alpha^2}{2\hbar^2}. \tag{9.34}$$

For the scattering states $E>0$

$$\psi''(x) = -k^2\psi(x); \qquad k = \frac{\sqrt{2mE}}{\hbar}, \tag{9.35}$$

and the general solution for $x<0$ is

$$\psi(x) = A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx}, \tag{9.36}$$

and for $x>0$

$$\psi(x) = F\mathrm{e}^{\mathrm{i}kx} + G\mathrm{e}^{-\mathrm{i}kx}. \tag{9.37}$$

Continuity requires that $F+G=A+B$ and

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \begin{cases} \mathrm{i}k\left(F\mathrm{e}^{\mathrm{i}kx} - G\mathrm{e}^{-\mathrm{i}kx}\right), & \text{for } x>0, \text{ so } \frac{\mathrm{d}\psi}{\mathrm{d}x}\big|_{+} = \mathrm{i}k\,(F-G)\,; \\ \mathrm{i}k\left(A\mathrm{e}^{\mathrm{i}kx} - B\mathrm{e}^{-\mathrm{i}kx}\right), & \text{for } x<0, \text{ so } \frac{\mathrm{d}\psi}{\mathrm{d}x}\big|_{-} = \mathrm{i}k\,(A-B)\,, \end{cases} \tag{9.38}$$

which gives the jump

$$\Delta\psi'\big|_{x=0} = \mathrm{i}k\,(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}\psi(0). \tag{9.39}$$

Because the plane waves are not normalizable in free space, these equations do not have unique solutions. Instead, we may assume a wave coming from a given direction, e.g. from left to right, see Fig. 9.4.

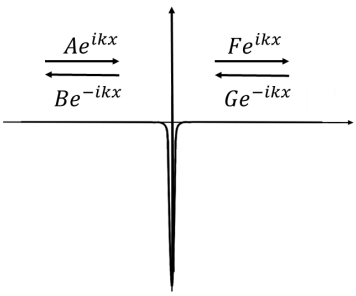

Figure 9.4: Directions for the given waves.

Thus assuming $G = 0$ gives B and F as a function of A

$$B = \frac{\mathrm{i}\beta}{1 - \mathrm{i}\beta}A \qquad F = \frac{1}{1 - \mathrm{i}\beta}A \tag{9.40}$$

$$\beta := \frac{m\alpha}{\hbar^2 k}. \tag{9.41}$$

These equations can be used to express the corresponding reflection and transmission probabilities $R + T = 1$

$$R := \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} \qquad T := \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}. \tag{9.42}$$

9.4 Scattering Matrix

The results based on specific potentials can be generalized to incoming and outgoing waves for any potential shape which can be divided into zero and non-zero regions (see Fig. 9.5).

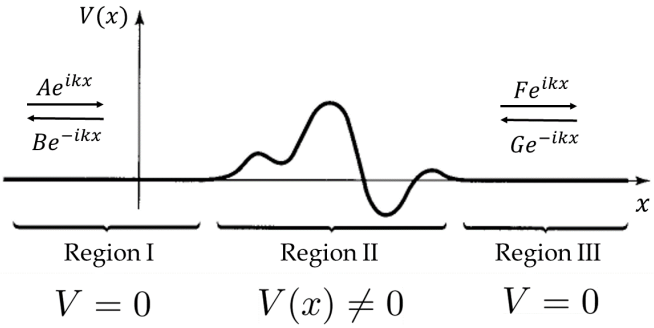

Figure 9.5: An example potential with zero and non-zero regions.

For the scattering sites $E > 0$

$$\psi''(x) = -k^2\psi(x), \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}, \tag{9.43}$$

and the general solutions for $V = 0$ are as above shown in Eqs. (9.36) and (9.37). The solution in between (Region II in Fig. 9.5) has some for that we do not define here explicitly, but instead we assume

that the Schrödinger equation can be solved in this region together with the the boundary conditions for continuity.

There are four boundary conditions that can be used to give[1] B and F in terms of A and G:

$$B = S_{11}A + S_{12}G; \tag{9.44}$$
$$F = S_{21}A + S_{22}G, \tag{9.45}$$

1: Two boundary conditions are consumed to determine the solution in Region II in terms of the other parameters, and hence there are two left to relate B and F to A and G.

It is suggestive to build up a 2×2 matrix.

$$\mathrm{S} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}, \tag{9.46}$$

which is the scattering (S) matrix, for which

$$\begin{bmatrix} B \\ F \end{bmatrix} = \mathrm{S} \begin{bmatrix} A \\ G \end{bmatrix}. \tag{9.47}$$

For scattering from the left, $G = 0$:

$$R_{\mathrm{l}} = \frac{|B|^2}{|A|^2}\Big|_{G=0} = |S_{11}|^2; \qquad T_{\mathrm{l}} = \frac{|F|^2}{|A|^2}\Big|_{G=0} = |S_{21}|^2, \tag{9.48}$$

and from the right, $A = 0$:

$$R_{\mathrm{r}} = \frac{|F|^2}{|G|^2}\Big|_{A=0} = |S_{22}|^2; \qquad T_{\mathrm{r}} = \frac{|B|^2}{|G|^2}\Big|_{A=0} = |S_{12}|^2. \tag{9.49}$$

Correspondingly, the complex-valued matrix elements S_{11} and S_{22} are referred to as the reflection coefficients and S_{12} and S_{12} are transmission coefficients.

Lecture 10 | 10

In quantum mechanics there are very few systems that can be exactly analytically solved. If one can justify that the system under study can be approximated by a solvable case which has been only slightly perturbed, it is possible to develop a systematic expansion of the full solution in terms of the eigenstates and energies of the solvable system. This is the basis of perturbation theory, which we consider in this chapter in the case where the Hamiltonians do not depend on time.

10.1 Intended learning outcomes

- Apply inner product to form an orthonormal basis from any complete set of eigenfunctions
- Apply perturbation theory to obtain accurate approximations for the eigenenergies and eigenstates of a Hamiltonian that is close to a solvable Hamiltonian

10.2 Time-Independent Non-Degenerate Perturbation Theory

Our problem is to find the eigenstates $\{\} |\psi_n\rangle\}$ and eigenenergies $\{E_n\}$ of a Hamiltonian

$$\hat{H} = \hat{H}^0 + \hat{H}', \tag{10.1}$$

where $\hat{H}'$ is a small perturbation to the exactly solvable Hamiltonian $\hat{H}^0$. We assume that all eigenvalues $\{E_n^0\}_n$ of $\hat{H}^0$ are non-degenerate, i.e., there is only a single linearly independent eigenstate for a given eigenvalue. Thus, the Schrödinger equation

$$\hat{H}^0 |\psi_n^0\rangle = E_n^0 |\psi_n^0\rangle, \tag{10.2}$$

naturally yields an orthonormal basis

$$\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm}. \tag{10.3}$$

Our original problem corresponds to solving

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle, \tag{10.4}$$

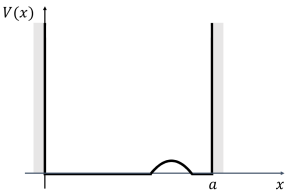

Figure 10.1: Small perturbation on $V(x)$.

which assume is difficult to do directly in an analytic manner. To proceed, we instead consider that by continuously adding the perturbation Hamiltonian $\hat{H}'$ to $\hat{H}^0$ the eigenenergies and eigenstates of $\hat{H}$ begin to continuously deviate from those of $\hat{H}'$. Thus, in the following, we consider a series expansion of $\{\} |\psi_n\rangle\}$ and $\{E_n\}$ in terms of $\{\} |\psi_n^0\rangle\}$ and eigenenergies $\{E_n^0\}$.

For the sake of carrying out the expansion, we write

$$\hat{H} = \hat{H}^0 + \lambda \hat{H}', \tag{10.5}$$

where now λ can be considered a small parameter to obtain the coefficients of the expansion, but in the end, we set $lambda = 1$. Consequently, we expand

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \lambda^2 |\psi_n^2\rangle + \cdots \tag{10.6}$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots , \tag{10.7}$$

where the superscripts denote the nth order corrections to the unperturbed state denoted by 0. This expression is inserted into Eq. (10.4) to obtain

$$\hat{H}^0 |\psi_n^0\rangle + \lambda \left(\hat{H}^0 |\psi_n^1\rangle + \hat{H}' |\psi_n^0\rangle \right) + \lambda^2 \left(\hat{H}^0 |\psi_n^2\rangle + \hat{H}' |\psi_n^1\rangle \right) + \cdots \tag{10.8}$$

$$= E_n^0 |\psi_n^0\rangle + \lambda \left(E_n^0 |\psi_n^1\rangle + E_n^1 |\psi_n^0\rangle \right) + \lambda^2 \left(E_n^0 |\psi_n^2\rangle + E_n^1 |\psi_n^1\rangle + E_n^2 |\psi_n^0\rangle \right) + \cdots . \tag{10.9}$$

Since this equation needs to be fulfilled by all values of λ at least in the limit $\lambda \to 0$, it actually needs to be fulfilled for all powers of λ individually.

The terms independent of λ yield just the Schrödinger equation for $\hat{H}_0$ which is satisfied by definition. To first order in λ, we obtain

$$\hat{H}^0 |\psi_n^1\rangle + \hat{H}' |\psi_n^0\rangle = E_n^0 |\psi_n^1\rangle + E_n^1 |\psi_n^0\rangle , \tag{10.10}$$

and to second order

$$\hat{H}^0 |\psi_n^2\rangle + \hat{H}' |\psi_n^1\rangle = E_n^0 |\psi_n^2\rangle + E_n^1 |\psi_n^1\rangle + E_n^2 |\psi_n^0\rangle . \tag{10.11}$$

Taking the inner product of the first equation with $|\psi_n^0\rangle$ gives the first-order correction as

$$E_n^1 = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle . \tag{10.12}$$

Although it is not trivial to see, this first-order correction of the energy can only be applied if the energy E_n^0 is non-degenerate as assumed above. We consider the degenerate in the following

sections, but the results of this section can only be applied in the non-degenerate case.

Rewriting the equation for the first-order correction as

$$\left(\hat{H}^0 - E_n^0\right)|\psi_n^1\rangle = -\left(\hat{H}' - E_n^1\right)|\psi_n^0\rangle\,, \tag{10.13}$$

and expanding $|\psi_n^1\rangle = \sum_m c_{m\neq n}^{(n)}|\psi_m^0\rangle$ gives

$$\sum_{m\neq n}\left(E_m^0 - E_n^0\right)c_m^{(n)}\,|\psi_m^0\rangle = -\left(\hat{H}' - E_n^1\right)|\psi_n^0\rangle\,. \tag{10.14}$$

Above, we have used $c_m^m = 0$ since otherwise the norm of $|\psi_n\rangle$ would depend on λ down to the first order. Taking the inner product with $|\psi_l^0\rangle$

$$\sum_{m\neq n}\left(E_m^0 - E_n^0\right)c_m^{(n)}\langle\psi_l^0|\psi_m^0\rangle = -\langle\psi_l^0|\hat{H}'|\psi_n^0\rangle + E_n^1\langle\psi_l^0|\psi_n^0\rangle, \tag{10.15}$$

and orthogonality gives

$$c_m^{(n)} = \frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}. \tag{10.16}$$

Thus the first-order correction to the eigensates is given by

$$|\psi_n^1\rangle = \sum_{m\neq n}\frac{\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle}{E_n^0 - E_m^0}\,|\psi_m^0\rangle\,. \tag{10.17}$$

Typically one needs to only use the first-order perturbation theory to obtain the most significant correction to the unperturbed case, but if for example, for symmetry reasons, the first-order correction vanishes, one needs to consider the second-order perturbation theory. To obtain the second-order corrections, we use Eq. (10.11) and take an inner product with $|\psi_n^0\rangle$ to obtain

$$\langle\psi_n^0|\hat{H}^0|\psi_n^2\rangle + \langle\psi_n^0|\hat{H}'|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^2\rangle + E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2\langle\psi_n^0|\psi_n^0\rangle, \tag{10.18}$$

where

$$\langle\psi_n^0|\psi_n^1\rangle = \sum_{m\neq n}c_m^{(n)}\langle\psi_n^0|\psi_m^0\rangle = 0, \tag{10.19}$$

and thus

$$E_n^2 = \sum_{m\neq n}\frac{\left|\langle\psi_m^0|\hat{H}'|\psi_n^0\rangle\right|^2}{E_n^0 - E_m^0}, \tag{10.20}$$

where we used Eq. (10.17) for the last equality. With this technique, one may derive also the second-order correction to the eigenstates

of $\hat{H}$ and all higher-order corrections, but we cease our derivations at this point, and instead proceed to discuss the degenerate perturbation theory.

10.3 Gram–Schmidt Orthogonalization

Above, we assumed that the Hamiltonian $\hat{H}_0$ is non-degenerate, and hence its eigenstates are orthogonal by construction. However, not all useful Hamiltonians are degenerate, which means that for conveniency, we need a process to form an orthogonal set from possibly non-orthogonal set of eigenstates that correspond to a single eigenvalue.

To begin, we assume that we have a set of *linearly independent* ket vectors

$$S = \{|v_1\rangle, |v_2\rangle, \cdots, |v_n\rangle\}, \tag{10.21}$$

which spans a Hilbert space $\tilde{\mathcal{H}}$. Our goal is to create a new orthonormal set

$$S_\perp^N = \{|e_1\rangle, |e_2\rangle, \cdots, |e_n\rangle\}. \tag{10.22}$$

that also spans the space $\tilde{\mathcal{H}}$.

The following method is referred to as the Gram–Schmidt orthogonalization process. Next, we define a projection operator

$$\hat{P}_u \coloneqq \frac{|u\rangle\langle u|}{\langle u|u\rangle}. \tag{10.23}$$

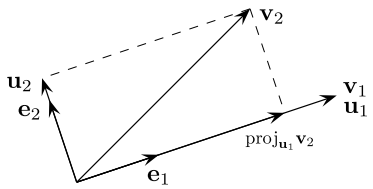

Figure 10.2: The first two steps of the Gram–Schmidt process [3].

The GS process simply comprises repeated orthogonal projections, subtracting the non-orthogonal parts and finally normalizing, see Fig. 10.2 as well:

$$|u_1\rangle = |v_1\rangle, \qquad |e_1\rangle = \frac{|u_1\rangle}{\|u_1\|}; \tag{10.24}$$

$$|u_2\rangle = |v_2\rangle - \hat{P}_{u_1}|v_2\rangle, \qquad |e_2\rangle = \frac{|u_2\rangle}{\|u_2\|}; \tag{10.25}$$

$$|u_3\rangle = |v_3\rangle - \hat{P}_{u_1}|v_3\rangle - \hat{P}_{u_2}|v_3\rangle, \qquad |e_3\rangle = \frac{|u_3\rangle}{\|u_3\|}; \tag{10.26}$$

$$|u_k\rangle = |v_k\rangle - \sum_{m=1}^{k-1} \hat{P}_{u_m}|v_k\rangle, \qquad |e_k\rangle = \frac{|u_k\rangle}{\|u_k\|}. \tag{10.27}$$

The final orthonormal basis set is

$$S_\perp^N = \{|e_1\rangle, |e_2\rangle, \cdots, |e_n\rangle\}, \tag{10.28}$$

which we can verify by noting that $\forall l < k \ \langle e_l|u_k\rangle = \langle e_l|v_k\rangle - \sum_{m=1}^{k-1} \langle e_l|e_m\rangle \langle e_m|v_k\rangle = 0 = \langle e_l|e_k\rangle = \langle e_k|e_l\rangle$.

10.4 Time-Independent Degenerate First-Order Perturbation Theory

The treatment in Sec. 10.2 does not work if the eigenenergy E_n^0 of $\hat{H}^0$ is degenerate, i.e., there are more than one linearly independent eigenstates that correspond to this eigenvalue. It turns out that each degenerate subspace can be handled independently up to the first-order perturbation theory. Thus, we consider $S = \{|\psi_{D,1}\rangle, |\psi_{D,2}\rangle, ..., |\psi_{D,k}\rangle\}$ to be a set of linearly independent eigenstates of $\hat{H}^0$ that satisfy

$$\hat{H}^0 |\psi_{D,i}\rangle = E_D |\psi_{D,i}\rangle, \ \forall i \in \{1, .., k\}. \tag{10.29}$$

Note that different eigenvectors of a Hermitian operator corresponding to the same eigenvalue need not necessarily be orthogonal. However, an orthonormal basis can be constructed through the Gram–Schmidt orthogonalization procedure described above. We assume here that the process has already been carried out such that the set S is orthonormal.

We define that the subspace $D \subset \mathcal{H}$ spanned by the basis S is a *degenerate subspace* of $\mathcal{H}$. Note that any state in this subspace is an eigenstate of $\hat{H}^0$ since

$$\hat{H}^0 \left(c_1 |\psi_{D,1}\rangle + c_2 |\psi_{D,2}\rangle + ... + c_n |\psi_{D,k}\rangle\right) \tag{10.30}$$

$$= E_D \left(c_1 |\psi_{D,1}\rangle + c_2 |\psi_{D,2}\rangle + ... + c_n |\psi_{D,k}\rangle\right), \ \forall c_i \in \mathbb{C}. \tag{10.31}$$

This implies that our choice of basis is not unique: any set of k orthonormal vectors in D is a possible choice. Thus, we expand the degenerate state $|\psi_n^0\rangle \in D$ as

$$|\psi_n^0\rangle = c_1 |\psi_{D,1}\rangle + c_2 |\psi_{D,2}\rangle + ... + c_n |\psi_{D,k}\rangle, \tag{10.32}$$

substitute it in the first-order equation (10.10), and take the inner product with one of our basis states, $|\psi_{D,i}\rangle$:

$$\langle\psi_{D,i}|\hat{H}^0|\psi_n^1\rangle + \langle\psi_{D,i}|\hat{H}'|\psi_n^0\rangle = \langle\psi_{D,i}|E_n^0|\psi_n^1\rangle + \langle\psi_{D,i}|E_n^1|\psi_n^0\rangle, \tag{10.33}$$

where $E_n^0 = E_D$. Since $\hat{H}$ is Hermitian, the first terms on each side cancel, and we are left with

$$\langle\psi_{D,i}|\hat{H}'|\psi_n^0\rangle = E_n^1 \langle\psi_{D,i}|\psi_n^0\rangle. \tag{10.34}$$

We proceed by inserting Eq. (10.32) above and obtain

$$\begin{aligned} &\langle\psi_{D,i}|\,\hat{H}'\left(c_1\,|\psi_{D,1}\rangle + c_2\,|\psi_{D,2}\rangle + \ldots + c_k\,|\psi_{D,k}\rangle\right) \\ &= E_n^1\,\langle\psi_{D,i}|\left(c_1\,|\psi_{D,1}\rangle + c_2\,|\psi_{D,2}\rangle + \ldots + c_k\,|\psi_{D,k}\rangle\right), \end{aligned} \tag{10.35}$$

which reduces into

$$c_1\,\langle\psi_{D,i}|\hat{H}'|\psi_{D,1}\rangle + c_2\,\langle\psi_{D,i}|\hat{H}'|\psi_{D,2}\rangle + \ldots + c_k\,\langle\psi_{D,i}|\hat{H}'|\psi_{D,k}\rangle = E_n^1 c_i \tag{10.36}$$

$$c_1 H'_{i1} + c_2 H'_{i2} + \ldots + c_k H'_{ik} = E_n^1 c_i, \tag{10.37}$$

where $H'_{\alpha\beta}$ are the matrix elements of $\hat{H}'$ in the basis S and the subscript D has been dropped for brevity. By considering the above equation for all i, we obtain a linear system of equations which can be expressed as an eigenvalue problem

$$\begin{bmatrix} H'_{11} & H'_{12} & . & . & . \\ H'_{21} & H'_{22} & . & . & . \\ . & & . & & \\ . & & & . & \\ . & & & & . \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ . \\ . \\ . \end{bmatrix} = E_n^1 \begin{bmatrix} c_1 \\ c_2 \\ . \\ . \\ . \end{bmatrix} \tag{10.38}$$

The eigenvalues of the above eigenvalue problem yield the first-order corrections to the energy E_n^0. Note that although we assumed E_n^0 to be degenerate, the degeneracy is typically lifted by the perturbation.

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Although the Schrödinger equation yields a complete solution to the corresponding problem at hand, the formulation of quantum dynamics for states and operators is not unique, but can be done in different ways. This does not of course change any of the underlying physics, but is more of technical value. The different formulations are referred to as *pictures* and they are the main topic in this chapter. First, the adiabatic theorem will be briefly mentioned and at the end the density operator will be introduced.

11.1 Intended learning outcomes

- Identify the adiabatic theorem
- Differentiate between Schrödinger, Heisenberg, and interaction pictures
- Apply the density operator to calculate expectation values and their evolution

11.2 Note on the adiabatic theorem

For the sake of brevity, we do not derive the adiabatic theorem here, but instead note its main result.

Assume that we have a system that very slowly evolves in time such that the Hamiltonian changes from $\hat{H}^{\mathrm{i}}$ to $\hat{H}^{\mathrm{f}}$, see Fig. 11.1 for an example.

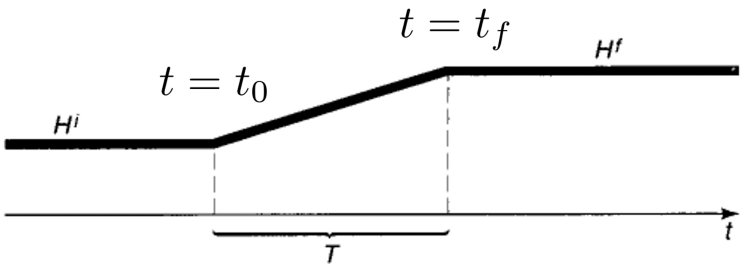

Figure 11.1: Hamiltonian changes from $\hat{H}^i$ to $\hat{H}^f$ in an interval $[t_0, t_{\mathrm{f}}]$ of length T. Provided that $1/T$ is much smaller than any transition frequency of the system during the ramp, the evolution is adiabatic.

Adiabatic processes carry the system from an initial eigenstate of $\hat{H}^{\mathrm{i}}$ to that of the final Hamiltonian $\hat{H}^{\mathrm{f}}$. In the case of level crossings, or degeneracies appearing or disappearing in the course of the evolution, the adiabaticity breaks down. If the spectrum says non-degenerate over the whole adiabatic evolution, one may simply

follow the continuous transformation of the eigenstates of $\hat{H}^{\mathrm{i}}$ to the corresponding eigenstates of $\hat{H}^{\mathrm{f}}$.

For example, if for the infinite well the wall distance is adiabatically increased from a to $2a$ (see Fig. 11.2):

$$\psi^{\mathrm{i}}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right) \quad \rightarrow \quad \psi^{\mathrm{f}}(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{\pi}{2a}x\right).$$

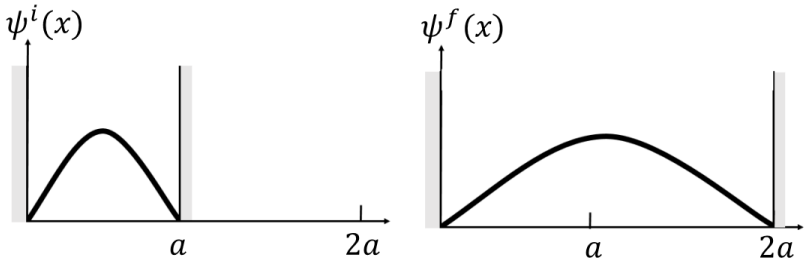

Figure 11.2: Increasing the width of an infinite potential well adiabatically deforms the initial ground state (on the left) into the final ground state (on the right).

For rapid non-adiabatic, or diabatic, processes the final state is some combination of final eigenstates.

Although usually in quantum mechanics an overall phase factor $\mathrm{e}^{\mathrm{i}\theta}$ is not measurable, a time-dependent Hamiltonian may make it possible to measure. Such a prefactor is referred to as the *Berry phase* and it is discussed in Appendix A.3.

11.3 Temporal dependence of operators

The *formulation of quantum dynamics is not unique for the states and operators*. Consider that we begin from an initial state $|\psi(0)\rangle$ and have a Hamiltonian $\hat{H}$ that yields the temporal evolution according to the Schrödinger equation. Thus the evolution of the expectation value of an operator $\hat{A}$ that does not itself depend explicitly on time is given by

$$\begin{aligned}
\langle\hat{A}\rangle(t) &= \langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\hat{U}(t)\psi(0)|\hat{A}|\hat{U}(t)\psi(0)\rangle \\
&= \langle\psi(0)|\hat{U}(t)^{\dagger}\hat{A}\hat{U}(t)|\psi(0)\rangle \\
&= \left(\psi(0)|\hat{U}^{\dagger}(t)\right)\hat{A}\left(\hat{U}(t)|\psi(0)\rangle\right) \\
&= \langle\psi(0)|\left(\hat{U}^{\dagger}(t)\hat{A}\hat{U}(t)\right)|\psi(0)\rangle, \qquad (11.1)
\end{aligned}$$

where we have used the results of Secs. 5.2 and 5.3 that the time-evolution operator arising from the Schrödinger equation propagates the state as

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi(0)\rangle\,, \qquad (11.2)$$

and follows the equation of motion

$$\mathrm{i}\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t} = \hat{H}(t)\hat{U}(t,t_0), \tag{11.3}$$

yielding

$$\hat{U}(t,t_0) = \mathcal{T}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}t'\hat{H}(t')}. \tag{11.4}$$

The form where the states evolve in time is referred to as the *Schrödinger picture*

$$\langle\hat{A}\rangle(t) = \Big(\langle\psi(0)|\hat{U}^\dagger(t)\Big)\,\hat{A}\Big(\hat{U}(t)|\psi(0)\Big), \tag{11.5}$$

and where the operators evolve in time but states stay the same is the *Heisenberg picture*:

$$\langle\hat{A}\rangle(t) = \langle\psi(0)|\,\Big(\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\Big)\,|\psi(0)\rangle. \tag{11.6}$$

Below, we define and discuss these pictures in more detail as well as introduce the *interaction picture* that lies between the Schrödinger and Heisenberg pictures.

11.4 Schrödinger Picture

The temporal evolution of all quantum states of the system described by $\hat{H}$ is governed by

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle_\mathrm{S} = \hat{H}|\psi(t)\rangle_\mathrm{S}, \tag{11.7}$$

or equivalently

$$|\psi(t)\rangle_\mathrm{S} = \hat{U}(t,0)|\psi(0)\rangle_\mathrm{S}. \tag{11.8}$$

Here the subscript S denotes and defines the quantum state in the Schrödinger picture which is the picture we have implicitly used in the above chapters. Thus for the states and operators, we have

$$|\psi(t)\rangle_\mathrm{S} = |\psi(t)\rangle \quad \text{and} \quad \hat{A}_\mathrm{S} = \hat{A}. \tag{11.9}$$

The evolution of the expectation value of the operator $\hat{A}$ is deter-

mined by

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial}{\partial t}\,{}_{\mathrm{S}}\langle\psi(t)|\hat{A}|\psi(t)\rangle_{\mathrm{S}} &= \mathrm{i}\hbar\left({}_{\mathrm{S}}\langle\psi(t)|\hat{A}|\dot{\psi}(t)\rangle_{\mathrm{S}} + {}_{\mathrm{S}}\langle\dot{\psi}(t)|\hat{A}|\psi(t)\rangle_{\mathrm{S}}\right) \\ &= {}_{\mathrm{S}}\langle\psi(t)|\hat{A}\hat{H}|\psi(t)\rangle_{\mathrm{S}} - {}_{\mathrm{S}}\langle\psi(t)|\hat{H}\hat{A}|\psi(t)\rangle_{\mathrm{S}} \\ &= \langle[\hat{A},\hat{H}]\rangle_{\mathrm{S}}. \end{aligned} \tag{11.10}$$

If the commutator is zero, the expectation value of $\hat{A}$ is a *constant of motion*.

11.5 Heisenberg picture

In the Heisenberg picture, the states do not evolve in time but the operators do. This arises from the definition

$$|\psi\rangle_{\mathrm{H}} = \hat{U}^{\dagger}(t,0)|\psi(t)\rangle_{\mathrm{S}} = \hat{U}^{\dagger}(t,0)\hat{U}(t,0)\,|\psi(0)\rangle_{\mathrm{S}} = |\psi(0)\rangle_{\mathrm{S}}\,, \tag{11.11}$$

which leads to the definition

$$\hat{A}_{\mathrm{H}}(t) = \hat{U}^{\dagger}(t,0)\hat{A}_{\mathrm{S}}\hat{U}(t,0), \tag{11.12}$$

since we wish that all expectation values are independent of the picture we are employing, see Eq.(11.1). Note that at $t = 0$, we have $\hat{A}_{\mathrm{H}}(0) = \hat{A}_{\mathrm{S}}(0)$.

The originally time-independent operators typically depend on time in the Heisenberg picture and their equation of motion is given by

$$\begin{aligned} \frac{\partial\hat{A}_{\mathrm{H}}}{\partial t} &= \partial_t\left(\hat{U}^{\dagger}\hat{A}_{\mathrm{S}}\hat{U}\right) \\ &= \frac{\mathrm{i}}{\hbar}\left(\hat{U}^{\dagger}\hat{H}\hat{A}_{\mathrm{S}}\hat{U} - \hat{U}^{\dagger}\hat{A}_{\mathrm{S}}\hat{H}\hat{U}\right) \\ &= \frac{\mathrm{i}}{\hbar}\left(\hat{H}_{\mathrm{H}}\hat{A}_{\mathrm{H}} - \hat{A}_{\mathrm{H}}\hat{H}_{\mathrm{H}}\right) \\ &= -\frac{\mathrm{i}}{\hbar}[\hat{A},\hat{H}]_{\mathrm{H}}. \end{aligned} \tag{11.13}$$

Note that for a time-independent Hamiltonian, the definition yields

$$\hat{H}_{\mathrm{H}} = \hat{U}^{\dagger}\hat{H}\hat{U} = \hat{H}, \tag{11.14}$$

but one should bear in mind that since the states $|\psi\rangle_{\mathrm{H}}$ are independent of time, the generator for their evolution vanishes, i.e., $\mathrm{i}\hbar\partial_t\,|\psi\rangle_{\mathrm{H}} = 0 \times |\psi\rangle_{\mathrm{H}} = 0$.

11.6 Interaction picture

As we noted above, the Schrödinger and Heisenberg pictures do not differ in any physics. when using the Schrödinger picture, one needs to solve the evolution of the quantum states according to $\hat{H}$ and in the Heisenberg picture one needs to track the temporal evolution of the operators according to $\hat{H}$. Thus at first glance, the two pictures seem equally challenging to use since they are both vested in the ability of exponentiate $\hat{H}$. In practice, it depends on the objectives which picture is more convenient. For example, if one needs to calculate the expectation value of a single operator, perhaps the Heisenberg picture is more convenient. If one is interested only on the evolution of the single quantum state, the Schrödinger picture may be advantageous. In general however, it does not depend on the picture whether the problem is fully analytically solvable or not, the use of the different pictures may simply reduce the workload needed in the calculations.

Taken this learning, let us consider a time-independent Hamiltonian $\hat{H}_\mathrm{S}$ and divide it into two parts as

$$\hat{H}_\mathrm{S} = \hat{H}_\mathrm{S}^{(0)} + \hat{H}_\mathrm{S}^\mathrm{I}, \tag{11.15}$$

where $\hat{H}_\mathrm{S}^{(0)}$ can be conveniently exponentiated. We proceed by defining the state vector in the *interaction picture* by

$$|\psi(t)\rangle_\mathrm{I} = \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}|\psi(t)\rangle_\mathrm{S}. \tag{11.16}$$

Note that this definition differs from the Heisenberg picture in that we do not cancel the whole temporal evolution of the state, but only aim to cancel the part of the evolution given by $\hat{H}_\mathrm{S}^{(0)}$.

Again, to keep the expectation values of operators independent of the used picture, operators $\hat{A}$ in the interaction picture are defined by

$$\hat{A}_\mathrm{I}(t) = \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}\hat{A}_\mathrm{S}\mathrm{e}^{-\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}. \tag{11.17}$$

Consequently, the Schrödinger equation in the interaction picture becomes

$$\begin{aligned}\mathrm{i}\hbar\partial_t|\psi(t)\rangle_\mathrm{I} &= -\hat{H}_\mathrm{S}^{(0)}\mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}|\psi(t)\rangle_\mathrm{S} + \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}\hat{H}_\mathrm{S}|\psi(t)\rangle_\mathrm{S} \\ &= \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}\hat{H}_\mathrm{S}^\mathrm{I}|\psi(t)\rangle_\mathrm{S} = \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}\hat{H}_\mathrm{S}^\mathrm{I}\mathrm{e}^{-\mathrm{i}\hat{H}_\mathrm{S}^{(0)}}\mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}}|\psi(t)\rangle_\mathrm{S} \\ &= \hat{H}_\mathrm{I}^\mathrm{I}(t)|\psi(t)\rangle_\mathrm{I},\end{aligned} \tag{11.18}$$

where $\hat{H}_\mathrm{I}^\mathrm{I}(t) = \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}\hat{H}_\mathrm{S}^\mathrm{I}\mathrm{e}^{-\mathrm{i}\hat{H}_\mathrm{S}^{(0)}}$. Thus we observe that, indeed, the Hamiltonian $\hat{H}_\mathrm{S}^{(0)}$ subtracts away from the Schrödinger equation,

though it still typically affects the temporal dependence of $\hat{H}_{\mathrm{I}}^{\mathrm{I}}(t)$. If $\hat{H}_{\mathrm{S}}^{(0)}$ and $\hat{H}_{\mathrm{S}}^{\mathrm{I}}$ commute, have have $\hat{H}_{\mathrm{I}}^{\mathrm{I}}(t) = \hat{H}_{\mathrm{S}}^{\mathrm{I}}$.

11.7 Density operator

Instead of ket vectors in the Hilbert space $\mathcal{H}$, quantum mechanics can also be formulated in the language of density operators. For a system in a quantum state $|\psi(t)\rangle$, the corresponding density operator $\hat{\rho}(t)$ is defined as

$$\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)| \,. \tag{11.21}$$

Consider any orthonormal basis $\{|n\rangle\}$ of $\mathcal{H}$, which yields the expansion

$$|\psi(t)\rangle = \sum_n c_n(t)\,|n\rangle \,. \tag{11.22}$$

In this basis, the density operator can be represented as a *density matrix* with the elements given by

$$\rho_{n,m}(t) = \langle n|\,\hat{\rho}(t)\,|m\rangle = \langle n|\psi\rangle\,\langle\psi|m\rangle = c_n(t)c_m^*(t). \tag{11.23}$$

On the other hand, the expectation value of an operator $\hat{A}$ in the state $|\psi(t)\rangle$ is

$$\langle\hat{A}(t)\rangle = \langle\psi|\hat{A}|\psi\rangle = \sum_{n,m} c_n(t)c_m^*(t)\,\langle m|\,\hat{A}\,|n\rangle = \sum_{n,m} A_{m,n}\rho_{n,m}(t), \tag{11.24}$$

where $A_{m,n}$ are the matrix elements of $\hat{A}$ in the chosen basis. This sum is the sum of the diagonal elements of the product matrix $A\rho$. This observation yields an important result

$$\langle\hat{A}\rangle(t) = \mathrm{Tr}\left[\hat{A}\hat{\rho}(t)\right] . \tag{11.25}$$

The density operator is particularly useful in describing statistical ensembles of quantum states, which can arise when the system contains unknown or untrackable degrees of freedom. In such a case, the defition of the density operator is extended to

$$\hat{\rho}(t) = \sum_i p_i\,|\psi_i\rangle\langle\psi_i| \,, \tag{11.26}$$

which for $\langle\psi_n|\psi_m\rangle = \delta_{nm}$ can be interpreted as the system being in each sate $|\psi_i\rangle \in \mathcal{H}$ with the classical probability $1 \geq p_i \geq 0$. The states described by density operators of the form of Eq. (11.21) are

Trace

$\mathrm{Tr}(\cdot)$ denotes the trace. The trace of an operator is equal to the sum of its diagonal entries in any matrix representation of the operator. In other words, for any operator $\hat{A} \in \mathcal{L}(\mathcal{H})$, we define

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle n|\,\hat{A}\,|n\rangle \,, \tag{11.19}$$

where $\{|n\rangle\}_n$ is any otrhonormal basis of the Hilbert space $\mathcal{H}$.

It follows that

$$\begin{aligned}\mathrm{Tr}(\hat{A}\hat{B}) &= \sum_n \langle n|\,\hat{A}\hat{B}\,|n\rangle \\ &= \sum_{n,m} \langle n|\,\hat{A}\,|\tilde{m}\rangle\langle\tilde{m}|\,\hat{B}\,|n\rangle \\ &= \sum_n \langle\tilde{n}|\,\hat{B}\hat{A}\,|\tilde{n}\rangle \\ &= \mathrm{Tr}(\hat{B}\hat{A}),\end{aligned} \tag{11.20}$$

where $\{|\tilde{m}\rangle\}_m$ is an otrhonormal basis of $\mathcal{H}$ which is possibly but not necessarily different from $\{|n\rangle\}_n$. Using such a different basis above also confirms the fact that the trace is independent of the choice of the basis used to compute it.

referred to as *pure states* and state, for which the sum in Eq. (11.26) has multiple non-vanishing terms, are referred to as *mixed states*. Even for mixed states, we employ Eq. (11.25) to compute the expectation value of operators.

Properties of the density operator:

- It is Hermitian, $\hat{\rho}^\dagger = \hat{\rho}$
- It is normalized, $\mathrm{Tr}\,\hat{\rho}(t) = 1$
- It is bound by pure states in the following sense: $\mathrm{Tr}[\hat{\rho}^2(t)] = 1$ for pure states and $\mathrm{Tr}[\hat{\rho}^2(t)] < 1$ for mixed states
- For mixed states, the elements of the density matrix are

$$\rho_{n,m} = \langle n|\hat{\rho}|m\rangle = \sum_i p_i \langle n|\psi_i\rangle\langle\psi_i|m\rangle \tag{11.27}$$

$$= \sum_i p_i c_n^{(i)} \left[c_m^{(i)}\right]^* . \tag{11.28}$$

Here, the density matrix elements represent the *eigenstate coefficients averaged over the mixture*. The n:th diagonal element of the density matrix is equal to the probability of occupying the quantum state $|n\rangle$, *i.e.*, to the populations. The off-diagonal elements are in general complex-valued and arise from the quantum superposition of the states $\{|\psi_k\rangle\}_k$ in the basis $\{|m\rangle\}_m$.

Temporal evolution of the density operator

Using the Schrödinger equation, one may show that (derivation is left as an exercise)

$$\frac{\partial\hat{\rho}(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar}[\hat{H},\hat{\rho}], \tag{11.29}$$

which is the famous *Liouville-von Neumann* equation. Its formal solution is

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t), \tag{11.30}$$

where the time evolution operator is defined as in Eq. (11.4).

The average of an operator $\hat{A}$ can be computed either in the Schrödinger picture (propagating the density operator) or in the Heisenberg picture (propagating $\hat{A}$):

$$\begin{aligned}\langle\hat{A}\rangle(t) &= \mathrm{Tr}\left(\hat{A}\hat{\rho}(t)\right)\\ &= \mathrm{Tr}\left(\hat{A}\hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)\right)\\ &= \mathrm{Tr}\left(\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\hat{\rho}(0)\right) \qquad (11.31)\\ &= \mathrm{Tr}\left(\hat{A}_\mathrm{H}(t)\hat{\rho}(0)\right), \qquad (11.32)\end{aligned}$$

where in Eq. (11.31), we have used the cyclic property of the trace: $\mathrm{Tr}\left(\hat{A}\hat{B}\hat{C}\right) = \mathrm{Tr}\left(\hat{C}\hat{A}\hat{B}\right) = \mathrm{Tr}\left(\hat{B}\hat{C}\hat{A}\right)$, which follows from the above-derived property $\mathrm{Tr}\left(\hat{A}\hat{B}\right) = \mathrm{Tr}\left(\hat{B}\hat{A}\right)$.

For a time-independent Hamiltonian the dynamics of the density matrix become

$$\rho_{n,m}(t) = \langle n|\hat{\rho}(t)|m\rangle = \langle n|\hat{U}(t)|\psi(0)\rangle\langle\psi(0)|\hat{U}^\dagger(t)|m\rangle. \tag{11.33}$$

If the chosen basis is the eigenbasis of the Hamiltonian, i.e., $|n\rangle$ and $|m\rangle$ are eigenstates of energy, we have

$$\hat{U}(t)\,|n\rangle = \mathrm{e}^{-\mathrm{i}E_n t/\hbar}\,|n\rangle\,, \tag{11.34}$$

and hence

$$\rho_{n,m}(t) = \mathrm{e}^{-\mathrm{i}(E_n-E_m)t/\hbar}\,\langle n|\psi(0)\rangle\,\langle\psi(0)|m\rangle = \mathrm{e}^{-\mathrm{i}(E_n-E_m)t/\hbar}\rho_{n,m}(0). \tag{11.35}$$

This implies that in the eigenbasis of energy, the populations are time-independent but the off-diagonal terms oscillate in time with a frequency corresponding to the level splitting. Thus also the absolute values of the off-diagonal elements are independent of time in the eigenbasis of energy and exhibit the coherent quantum superposition between the different eigenstates of energy. If the off-diagonal elements are zero, there is no superposition, but we have merely a classical probability of being in the different states. Thus the coherence of the state is associated to the persistence of the off-diagonal elements and the decay of these elements, for example owing to interaction of the system with its environment, is referred to as *decoherence*. In fact, also energy decay of the system leads to decoherence since a pure eigenstate of energy has no off-diagonal elements in the eigenbasis of energy. To differentiate the effects in excess of energy decay, the pure loss of phase coherence where the effect of ther energy decay is subtracted is referred to as *pure dephasing*.

Density operator in the interaction picture

In the interaction picture, we express the Hamiltonian as in Eq. (11.15) as

$$\hat{H}_\mathrm{S} = \hat{H}_\mathrm{S}^{(0)} + \hat{H}_\mathrm{S}^\mathrm{I}, \tag{11.36}$$

and the evolution of the state vector is given by Eq. (11.16) as

$$|\psi(t)\rangle_\mathrm{I} = \mathrm{e}^{\mathrm{i}\hat{H}_\mathrm{S}^{(0)}t/\hbar}|\psi(t)\rangle_\mathrm{S} =: \hat{U}_0^\dagger(t)|\psi(t)\rangle_\mathrm{S}. \tag{11.37}$$

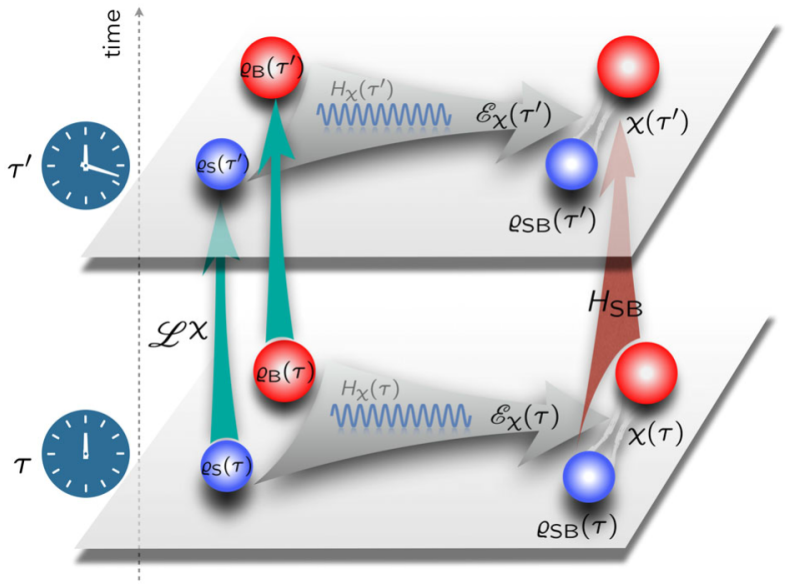

Figure 11.3: Description of the correlation picture. At any time τ (or τ_0), a correlating transformation $\mathcal{E}_\chi$ transforms an uncorrelated state $\varrho_S \otimes \varrho_B$ to a correlated state $\varrho_{SB} = \varrho_S \otimes \varrho_B + \chi$, at the same instant of time, due to an abstract correlation-dependent parent operator given by H_χ. Using this transformation, we obtain the temporal evolution of the uncorrelated system with a universal Lindblad-like generator $\mathcal{L}^\chi$ constructed from H_{SB}, the generator of the total system dynamics in the Schrödinger picture.

Thus the density operator in the interaction picture is defined as

$$\hat{\rho}_I(t) = \hat{U}_0^\dagger(t)\rho_S\hat{U}_0(t). \tag{11.38}$$

In analogy to the case of the interaction picture with the ket vectors, the equation of motion for $\hat{\rho}_I^I$ becomes

$$\frac{\partial\hat{\rho}_I(t)}{\partial t} = -\frac{i}{\hbar}[\hat{H}_I^I(t), \hat{\rho}_I(t)], \tag{11.39}$$

where $\hat{H}_I^I(t) = \hat{U}_0(t)\hat{H}_S^I\hat{U}_0^\dagger(t)$.

Correlation picture

Recently, a correlation picture has been introduced for open quantum systems [4], see Fig. 11.3, but we do not consider it in this course.

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Appendix A

The appendix contains some interesting extra topics that could not be discussed during the course.

A.1 Eigenstates of energy for the quantum harmonic oscillator using the position basis representation of the Schrödinger equation

For completeness, we introduce in this section another way of solving for the eigenfunctions and values of the QHO, based on writing the Schrödinger equation in the coordinate basis.[1] In Sec. 7.5, we derived the time-dependent Schrödinger equation in the position basis, and consequently, we obtain the corresponding time-dependent equation by the ansatz $\psi(x,t) = \exp(-iEt/\hbar)\psi(x)$ as

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \frac{m\omega^2}{2}x^2\psi(x) = E\psi(x). \tag{A.1}$$

1: We go through the derivation in a compact way, and hence we do not require you to be able to do the derivation in the exam, but it is good to remember the end result.

To simplify the equation, it is useful to define

$$q = \sqrt{\frac{m\omega}{\hbar}}x, \qquad \lambda = \frac{2E}{\hbar\omega}, \qquad \psi(x) = u\left(\sqrt{m\omega/\hbar}x\right) = u(q), \tag{A.2}$$

which gives

$$\frac{\mathrm{d}^2u}{\mathrm{d}q^2} + (\lambda - q)^2\, u = 0. \tag{A.3}$$

This is an inhomogeneous but linear differential equation which can be solved in multiple ways. The easiest is to write $u(q)$ as[2]

$$u(q) = H(q)\mathrm{e}^{-q^2/2}, \tag{A.4}$$

2: Note that here H does not denote the Hamiltonian but is instead a temporary symbol for a function that we aim to solve.

where the functions $H(q)$ satisfy the differential equation

$$H'' - 2qH' + (\lambda - 1)\, H = 0. \tag{A.5}$$

The solutions of Eq. (A.5) are polynomial Hermite functions of order n that can be explicitly constructed by assuming that the Hermite functions have a (polynomial) power law expansion, which is then inserted in Eq. (A.5). Matching terms with equal

powers in the expansion inserted in Eq. (A.5) requires that $\lambda = 2n+1$ with n being an integer, which gives

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right). \tag{A.6}$$

The Hermite polynomials can be generated through

$$H_n(y) = (-1)^n \mathrm{e}^{y^2} \frac{\mathrm{d}^n}{\mathrm{d}y^n} \mathrm{e}^{-y^2}. \tag{A.7}$$

The complete, normalized eigenfunctions of the QHO are given by

$$\psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!}\right) H_n(\alpha x) \mathrm{e}^{-\alpha^2 x^2/2}, \tag{A.8}$$

where $\alpha = \sqrt{m\omega/\hbar}$. The eigenfunctions are shown in Fig. 7.1. Figure 7.2 further demonstrates the potential energy and the probability density for finding the particle at a given point. In the figures, $\xi = q = \alpha x$.

The importance of the Hermite functions is that they form a *complete, orthogonal set of polynomial eigenfunctions in the Hilbert space*, where the *weighted* inner product is defined by

$$\int_{-\infty}^{\infty} H_n(\xi) H_k(\xi) \mathrm{e}^{-\xi^2} \mathrm{d}\xi = 0, \qquad \text{for } n \neq k. \tag{A.9}$$

The inner product between the eigenstates that form a complete orthonormal basis of the Hilbert space $\mathcal{H}$ is given by

$$(|\psi_n\rangle, |\psi_k\rangle) \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, \psi_n^*(x) \psi_k(x) = \delta_{nk}, \tag{A.10}$$

where the wave functions of the eigenstates are expressed as

$$\psi_n(x) = 2^{-\frac{n}{2}} (n!)^{-\frac{1}{2}} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right). \tag{A.11}$$

A.2 Particle in a square-well potential

Another simple but less trivial example is that of a quantum particle in a one-dimensional *square-well potential* (Fig. A.1):

$$V(x) = \begin{cases} \infty, & \text{if } -\infty \leq x \leq 0; \\ -V_0, & \text{if } 0 \leq x \leq a, \\ 0, & \text{if } a \leq x \leq \infty. \end{cases} \tag{A.12}$$

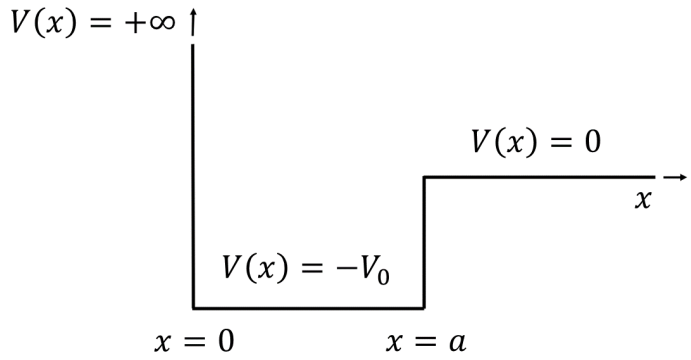

Figure A.1: Square-well potential.

We consider this example since it turns out below that there are two types of eigenstates of the Hamiltonian: *bound* states that are localized in the potential well with negative energy in reference to the zero level of the potential and *unbound* states that extent to infinity with positive energy.

First we note that for $x < 0$, $\psi(x) = 0$ as in the previous section since the potential is infinitely strong for $x < 0$. For $0 < x < a$, the time-independent Schrödinger equation yields

$$\psi''(x) = -k_0^2\psi(x); \qquad E = \frac{\hbar^2 k_0^2}{2m} - V_0, \tag{A.13}$$

with the solution $\psi(x) = C\sin(k_0 x)$. Thus for $0 < x < a$, the solution looks identical to that of the infinite-well case, but here the momentum, or wave number, is modified by the potential.

In the region, $x > a$, the free-particle solution applies:

$$\psi''(x) = k^2\psi(x); \qquad k^2 = -\frac{2mE}{\hbar^2}. \tag{A.14}$$

At this point, we restrict our considerations first to the case of negative energies, $E < 0$. Thus, $k \in \mathbb{R}$ in Eq. (A.14) which has the general solution $\psi(x) = Ae^{-kx} + Be^{kx}$. Next, we choose $k \geq 0$ and hence $B = 0$ since otherwise the wave function would diverge at large x.

The continuity of $\psi(a)$ and $\psi'(a)$ requires that

$$\begin{aligned} C\sin(k_0 a) &= Ae^{-ka}, \\ Ck_0\cos(k_0 a) &= -Ake^{-ka}, \end{aligned} \tag{A.15}$$

respectively. Hence, we must have

$$k_0\cot(k_0 a) = -k. \tag{A.16}$$

Because both variables depend on the energy E according to Eqs. (A.13) and (A.14), they have to satisfy

$$k^2 + k_0^2 = \frac{2V_0 m}{\hbar^2}. \tag{A.17}$$

For these bound states to exist, these two equations have to match as illustrated in Fig. A.2.

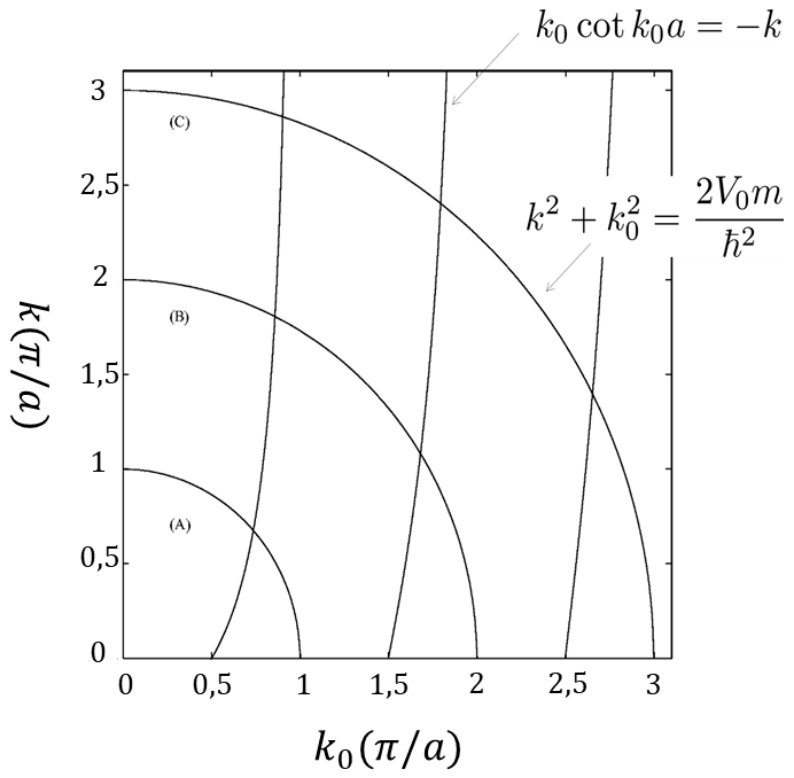

Figure A.2: Allowed parameters for bound states.

Let us next consider the case $E > 0$ which leads to the unbound states. The wave function is again zero for $x < 0$. For $0 < x < a$, we again have the solution $\psi(x) = C \sin(k_0 x)$ according to Eq. (A.13). In the region $a < x < \infty$,

$$\psi''(x) = -k^2 \psi x; \qquad E = \frac{\hbar^2 k^2}{2m}, \tag{A.18}$$

and the solution becomes a sum of a since and cosine term, which we express as

$$\psi(x) = D \sin(kx + \delta), \tag{A.19}$$

where $D, \delta \in \mathbb{R}$ are the constants to be determined by the boundary conditions.

Thus, the continuity of $\psi(a)$ and $\psi'(a)$ yields

$$k_0 \cot(k_0 a) = k \cot(ka + \delta). \tag{A.20}$$

Unlike for the bound states, there is a smooth eigenfunction for any energy $E > 0$, of the form

$$\psi(x) = \begin{cases} 0, & \text{if } -\infty < x < 0; \\ C \sin k_0 x, & \text{if } 0 < x < a; \\ D \sin(kx + \delta), & \text{if } a < x < \infty. \end{cases} \tag{A.21}$$

By defining

$$A_0 = -\frac{C}{2\mathrm{i}} \quad \text{and} \quad A = -\frac{D\mathrm{e}^{-2\mathrm{i}\delta}}{2\mathrm{i}} \tag{A.22}$$

we can write the solutions in the form

$$\psi(x) = \begin{cases} \overbrace{A_0 \mathrm{e}^{-\mathrm{i}k_0 x} - A_0 \mathrm{e}^{+\mathrm{i}k_0 x}}^{\text{wave traveling back and forth inside the well}}, & \text{if } 0 < x < a; \\ \underbrace{A\mathrm{e}^{-\mathrm{i}kx}}_{\text{incoming wave}} - \underbrace{A\mathrm{e}^{2\mathrm{i}\delta}}_{\text{outgoing wave with phase difference } 2\delta} \mathrm{e}^{+\mathrm{i}kx}, & \text{if } a < x < \infty. \end{cases} \tag{A.23}$$

See Fig. A.3 with an example of a typical eigenfunction corresponding to an unbound state, with a phase shift and amplitude change due to the external potential.

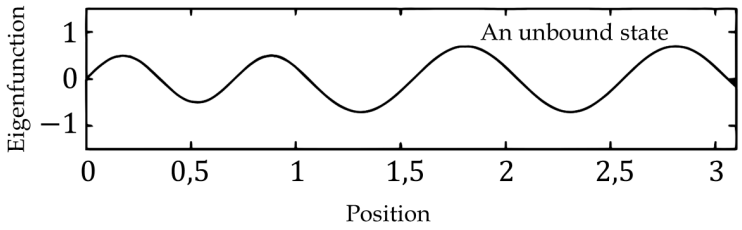

Figure A.3: Example wave function corresponding to an eigenstate of energy of an unbound state. The position is in units of the width of the square-well potential a.

A.3 Geometric and Berry Phases

If the Hamiltonian is independent of time, a particle that starts in the nth eigenstate

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \tag{A.24}$$

remains in that eigenstate and picks up a phase factor from the Schrödinger equation

$$\Psi_n(x,t) = \psi_n(x)\mathrm{e}^{\frac{\mathrm{i}E_n t}{\hbar}}. \tag{A.25}$$

If the Hamiltonian is time dependent, we can formally write (but usually not solve)

$$\hat{H}(t)\psi_n(x,t) = E_n(t)\psi_n(x,t). \tag{A.26}$$

According to the adiabatic theorem (see Section 11.2), the system will remain at the nth eigenstate even with time dependence:

$$\psi_n(x,t) = \hat{U}(t)\psi_n(x,t) \tag{A.27}$$

To obtain the time-evolution operator for a *time-dependent Hamiltonian*, we have to solve for

$$\mathrm{i}\hbar\frac{\partial\hat{U}(t,t_0)}{\partial t} = \hat{H}(t)\hat{U}(t,t_0) \tag{A.28}$$

The formal solution of this equation for Hamiltonians commuting at all times is (prove by expanding the exp function)

$$\hat{U}(t,t_0) = \mathrm{e}^{-\mathrm{i}\int_{t_0}^{t}\mathrm{d}t'\hat{H}(t')/\hbar} \tag{A.29}$$

Operating on the eigenstates gives simply that

$$\Psi_n(x,t) = \psi_n(x,t)\mathrm{e}^{-\mathrm{i}\int_{t_0}^{t}\mathrm{d}t' E_n(t')/\hbar}\mathrm{e}^{\mathrm{i}\gamma_n(t)} \tag{A.30}$$

The term

$$\theta_n(x,t) = -\int_{t_0}^{t}\mathrm{d}t'\frac{E_n(t')}{\hbar} \tag{A.31}$$

Is known as the *dynamic phase* and the extra phase factor $\gamma_n(t)$ is the *geometric phase*. We can plug in the solution back to the time-dependent SE to get

$$\mathrm{i}\hbar\left[\frac{\partial\psi_n}{\partial t}\mathrm{e}^{\mathrm{i}\theta_n}\mathrm{e}^{\mathrm{i}\gamma_n} - \frac{\mathrm{i}}{\hbar}E_n\psi_n\mathrm{e}^{\mathrm{i}\theta_n}\mathrm{e}^{\mathrm{i}\gamma_n} + \mathrm{i}\frac{\mathrm{d}\gamma_n}{\mathrm{d}t}\psi_n\mathrm{e}^{\mathrm{i}\theta_n}\mathrm{e}^{\mathrm{i}\gamma_n}\right] \tag{A.32}$$

$$= \left[\hat{H}\psi_n\right]\mathrm{e}^{\mathrm{i}\theta_n}\mathrm{e}^{\mathrm{i}\gamma_n} = E_n\psi_n\mathrm{e}^{\mathrm{i}\theta_n}\mathrm{e}^{\mathrm{i}\gamma_n} \tag{A.33}$$

and thus

$$\frac{\partial\psi_n}{\partial t} + \mathrm{i}\psi_n\frac{\mathrm{d}\gamma_n}{\mathrm{d}t} = 0. \tag{A.34}$$

Taking the inner product with ψ_n

$$\frac{\mathrm{d}\gamma_n}{\mathrm{d}t} = \mathrm{i}\langle\psi_n|\frac{\partial\psi_n}{\partial t}\rangle. \tag{A.35}$$

Let us assume that the time dependence in the Hamiltonian is

given by some (classical) function $R(t)$:

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R}\frac{\mathrm{d}R}{\mathrm{d}t} \quad \rightarrow \quad \frac{\mathrm{d}\gamma_n}{\mathrm{d}t} = \mathrm{i}\langle\psi_n|\frac{\partial \psi_n}{\partial R}\rangle\frac{\mathrm{d}R}{\mathrm{d}t}. \tag{A.36}$$

This can be integrated to give

$$\gamma_n(t) = \mathrm{i}\int_0^t \langle\psi_n|\frac{\partial \psi_n}{\partial R}\rangle\frac{\mathrm{d}R}{\mathrm{d}t'}\mathrm{d}t' = \mathrm{i}\int_{R_i}^{R_f}\langle\psi_n|\frac{\partial \psi_n}{\partial R}\rangle\mathrm{d}R. \tag{A.37}$$

If there are N time-dependent parameters in the Hamiltonian:

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1}\frac{\mathrm{d}R_1}{\mathrm{d}t} + \frac{\partial \psi_n}{\partial R_2}\frac{\mathrm{d}R_2}{\mathrm{d}t} + \cdots + \frac{\partial \psi_n}{\partial R_N}\frac{\mathrm{d}R_N}{\mathrm{d}t} \tag{A.38}$$

$$= (\nabla_R \psi_n)\cdot\frac{\mathrm{d}\vec{R}}{\mathrm{d}t}. \tag{A.39}$$

This can be again integrated to give

$$\gamma_n(t) = \mathrm{i}\int_{\vec{R}_i}^{\vec{R}_f}\langle\psi_n|\nabla_R\psi_n\rangle\cdot\mathrm{d}\vec{R}. \tag{A.40}$$

If the Hamiltonian is cyclic with period T

$$\gamma_n(T) = \mathrm{i}\oint\langle\psi_n|\nabla_R\psi_n\rangle\cdot\mathrm{d}\vec{R}. \tag{A.41}$$

This is a line integral around a closed loop in the parameter space and in general it is nonzero. $\gamma_n(t)$ is called the *Berry phase*.

The Berry phase only depends on the (adiabatic) path taken, not on time! In contrast, the dynamic phase is time dependent, as

$$\theta_n(T) = -\frac{1}{\hbar}\int_0^T E_n(t')\mathrm{d}t' \tag{A.42}$$

The Berry phase is *real-valued and it is measurable* [1]!

A.4 Time-dependent perturbation theory

A.5 Bloch's theorem

An important special case is that of a periodic potential $V(x+a) = V(x)$, see Fig. A.4.

Theorem A.5.1 (Bloch's theorem) *Any wave function that is a*

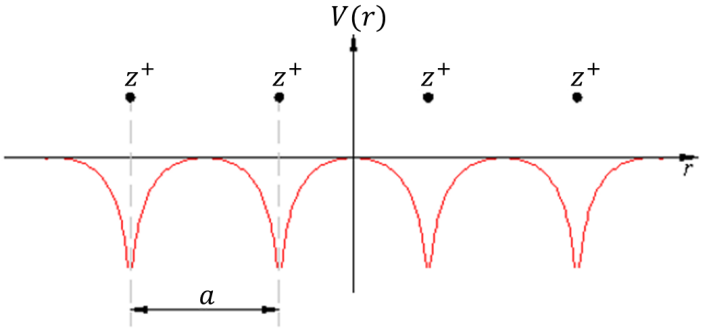

Figure A.4: Example of a periodic potential.

solution of the SE in a periodic potential must be of the form.

$$\psi(x) = e^{ikx}u(x)$$

where $u(x)$ *must satisfy* $u(x + a) = u(x)$ *and the wave vector is quantized as* $k = \frac{2\pi n}{L}$ *for* $n = 0, \pm 1, \cdots, \pm\frac{N}{2}$ *with* $L = Na$.

Bloch's theorem plays a central role in the theory of periodic crystalline materials, where for example the electronic states (electron wave functions) and phonon eigenstates (crystal vibrational eigenfunctions) must satisfy it. This leads to the concepts of electronic band structure (and phonon/vibrational bands) that exist in the Brillouin zone in k-space.

A.6 Bosons and Fermions

To make quantum statistics relevant, we need to consider more than just an isolated single particle. Consider first a two-particle wave function for identical particles $\Psi(x_1, x_2, t)$. The probability for finding particle 1 at dx_1 and particle 2 at dx_2 is given by

$$|\Psi(x_1, x_2, t)|^2 \, dx_1 dx_2. \tag{A.43}$$

If the particles are identical, they can be interchanged and thus

$$|\Psi(x_1, x_2, t)|^2 = |\Psi(x_2, x_1, t)|^2, \tag{A.44}$$

which means that

$$\Psi(x_1, x_2, t) = \Psi(x_2, x_1, t)e^{i\delta}, \tag{A.45}$$

where the phase factor $e^{i\delta} = \pm 1$. If we have a *Fock space* of identical single-particle wave functions, the symmetric and antisymmetric (entangled) wave functions can be represented as

$$\Psi^S(x) \propto \psi_n(x_1)\psi'_n(x_2) + \psi_n(x_2)\psi'_n(x_1); \tag{A.46}$$

$$\Psi^A(x) \propto \psi_n(x_1)\psi'_n(x_2) - \psi_n(x_2)\psi'_n(x_1). \tag{A.47}$$

Qualitatively, particles with antisymmetric (entangled) wave function avoid each other. We will next explicitly demonstrate this in the case of a 1D QHO.

Consider two particles in two different single-particle states in a 1D QHO, first one with n and the other one with n'. The energy is

$$E = E_n + E_{n'} = (n + n' + 1)\hbar\omega. \tag{A.48}$$

For two *distinguishable* particles, p and q, the total wave function can be of *unentangled* form:

$$\Psi_1^{(D)}(x_p, x_q, t) = \psi_n(x_p)\psi_{n'}(x_q)\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar}; \tag{A.49}$$

$$\Psi_2^{(D)}(x_p, x_q, t) = \psi_n(x_q)\psi_{n'}(x_p)\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar}, \tag{A.50}$$

or a linear combination as

$$\Psi^{(D)}(x_p, x_q, t) = c_1\Psi_1^{(D)}(x_p, x_q, t) + c_2\Psi_2^{(D)}(x_p, x_q, t). \tag{A.51}$$

This latter wave function (WF) is *entangled* because it associates both particles with both single-particle states.

For two *identical* particles there are two possible WFs as

$$\Psi^{(S)}(x_p, x_q, t) = \frac{1}{\sqrt{2}}\left[\psi_n(x_p)\psi_{n'}(x_q) + \psi_n(x_q)\psi_{n'}(x_p)\right]\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar}; \tag{A.52}$$

$$\Psi^{(A)}(x_p, x_q, t) = \frac{1}{\sqrt{2}}\left[\psi_n(x_p)\psi_{n'}(x_q) - \psi_n(x_q)\psi_{n'}(x_p)\right]\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar}. \tag{A.53}$$

Next, set particles to have identical positions $x_p = x_q = x_0$. The unentangled WF for distinguishable particles is

$$\Psi_{1,2}^{(D)}(x_0, x_0, t) = \psi_n(x_0)\psi_{n'}(x_0)\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar} \tag{A.54}$$

For two identical particles the symmetrical unentangled WF is

$$\Psi_{1,2}^{(S)}(x_0, x_0, t) = \sqrt{2}\psi_n(x_0)\psi_{n'}(x_0)\mathrm{e}^{-\mathrm{i}(E_n+E_{n'})t/\hbar} \tag{A.55}$$

and the antisymmetrical one

$$\Psi^{(A)}(x_0, x_0, t) = 0 \tag{A.56}$$

The physical reason for these differences is *constructive or destructive interference* of the WFs.

The physical differences become even more clear if we consider two identical or distinguishable (D) particles occupying 1D QHO

states with $n = 0$ and $n' = 1$, using reduced coordinates

$$x = x_p - x_q \quad \text{and} \quad X = \frac{x_p + x_q}{2}. \tag{A.57}$$

The corresponding WFs can be easily constructed (homework) and the probability density functions (PDF) are plotted in Fig. A.5 for the symmetrical (S) and antisymmetrical (A) WFs of two identical particles and (unentangled) distinguishable particles (D)

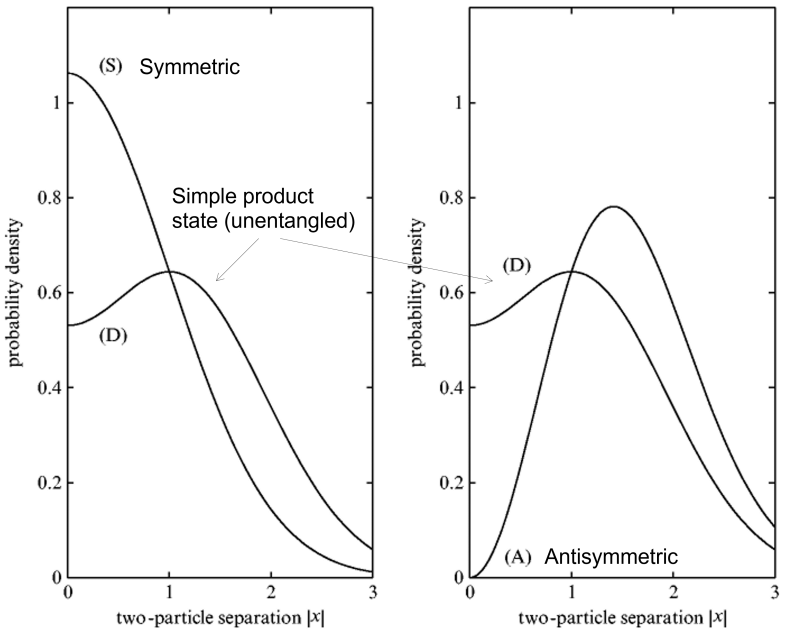

Figure A.5: Probability density functions for the 1D QHO in the symmetrical (S), antisymmetrical (A), and unentangled (D) cases.

Next we will just state the fundamental spin-statistics theorem. Proving it requires relativistic quantum field theory and will be presented in advanced quantum mechanics courses.

Theorem A.6.1 (Spin-statistics theorem) *There are two fundamental classes of particles: fermions with half-integer spin and bosons with integer spin*

- Fermions: quarks and composite particles made of them, and leptons such as the electron and neutrinos
- Bosons: Often force-mediating particles (photons, gluons, W and Z bosons, Higgs boson etc.), and composite particles (mesons)

Before discussing the symmetry of the wave functions, we should also note that there is a very simple rule for fermions: they cannot have identical wave functions, *i.e.*, they cannot have the exactly same set of quantum numbers. For example, if there are two electrons in the same energy eigenstate they must have opposite spin quantum numbers $s = \pm\frac{1}{2}$. Bosons, on the other hand, have

no such limitation which leads to the interesting phenomenon of *Bose condensation* in many physical systems with bosons.

Symmetrized Eigenstates for Bosons

For bosons the total wave function must be symmetric under the interchange of any degrees of freedom (coordinates) and any number of them can have the same quantum numbers.

Let us define a permutation operator $\hat{P}_{ij}$ by

$$\hat{P}_{ij}|k_1, k_2, \cdots, k_i, k_j, \cdots, k_N\rangle = |k_1, k_2, \cdots, k_j, k_i, \cdots, k_N\rangle. \quad \text{(A.58)}$$

Sum over all the permutations includes all possible combinations of the k's

$$\sum_{\hat{P}} \hat{P}|k_1, k_2, \cdots, k_N\rangle \coloneqq \sum \text{all } N! \text{ permutations of momenta in } |k_1, k_2, \cdots, k_N\rangle. \quad \text{(A.59)}$$

For example,

$$\sum_{\hat{P}} \hat{P}|k_1, k_2, k_3\rangle = \{|k_1, k_2, k_3\rangle + |k_2, k_1, k_3\rangle + |k_1, k_3, k_2\rangle \quad \text{(A.60)}$$
$$+ |k_3, k_2, k_1\rangle + |k_3, k_1, k_2\rangle + |k_2, k_3, k_1\rangle\}.$$

Since there can be any number of particles with the same k, we must count all possible combinations of different ways of organizing the ket:

$$n_i = \text{number of particles with momentum } k_i; \quad \text{(A.61)}$$
$$N = \sum_{i=1}^{N} n_i = \text{total number of particles.} \quad \text{(A.62)}$$

Thus there are exactly $\dfrac{N!}{\prod_{\alpha=1}^{N} n_\alpha!}$ different kets in $\sum_{\hat{P}} \hat{P}|k_1, k_2, \cdots, k_N\rangle$.
Using orthonormality of the basis functions

$$\langle k_a, k_b, \cdots, k_l|k'_a, k'_b, \cdots, k'_l\rangle = \delta_{k_a,k'_a}\delta_{k_b,k'_b} \times \cdots \times \delta_{k_l,k'_l}, \quad \text{(A.63)}$$

we can write the symmetrized, orthonormal N-body momentum eigenstate as

$$|k_1, k_2, \cdots, k_N\rangle^{(S)} = \left(\frac{N!}{\prod_{\alpha=1}^{N} n_\alpha!}\right) \sum_{\hat{P}} \hat{P}|k_1, k_2, \cdots, k_N\rangle, \quad \text{(A.64)}$$

which also form a complete, orthonormal set, with the identity operator

$$\hat{1}^{(S)} = \frac{1}{N!} \sum_{k_1,k_2,\cdots,k_N} \left(\prod_{\alpha=1}^{N} n_\alpha! \right) |k_1, k_2, \cdots, k_N\rangle^{(S)} \langle k_1, k_2, \cdots, k_N|^{(S)}. \tag{A.65}$$

Symmetrized Eigenstates for Fermions

For fermions the total wave function must be *antisymmetric* under the interchange of any degrees of freedom (coordinates) and none of them can have the same quantum numbers.

Let us again define a permutation operator $\hat{P}_{ij}$ as in Eq. (A.58). Likewise, sum over all the permutations includes all possible combinations of the wave vectors as in Eq. (A.59).

The antisymmetric momentum eigenstates can be written as

$$|k_1, k_2, \cdots, k_N\rangle^{(A)} = \frac{1}{\sqrt{N!}} \sum_{\hat{P}} (-1)^p \hat{P} |k_1, \cdots, k_N\rangle, \tag{A.66}$$

where p is the number of permutations (changes)

For example,

$$\sum_{\hat{P}} (-1)^p \hat{P} |k_1, k_2, k_3\rangle = \{|k_1, k_2, k_3\rangle - |k_2, k_1, k_3\rangle - |k_1, k_3, k_2\rangle \\ - |k_3, k_2, k_1\rangle + |k_3, k_1, k_2\rangle + |k_2, k_3, k_1\rangle\}. \tag{A.67}$$

An interesting special case is where we approximate the total N-body wave function with products of single-particle wave functions $\langle r_i|k_j\rangle$, in which case the total antisymmetric fermion wave function $\langle r_1, r_2, \cdots r_N|k_1, k_2, \cdots, k_N\rangle^{(A)}$ can be written as the *Slater determinant*

$$\langle r_1, r_2, \cdots r_N|k_1, k_2, \cdots, k_N\rangle^{(A)} = \frac{1}{\sqrt{N}} \begin{vmatrix} \langle r_1|k_1\rangle & \langle r_1|k_2\rangle & \cdots & \langle r_1|k_N\rangle \\ \langle r_2|k_1\rangle & \langle r_2|k_2\rangle & \cdots & \langle r_2|k_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle r_N|k_1\rangle & \langle r_N|k_2\rangle & \cdots & \langle r_N|k_N\rangle \end{vmatrix}, \tag{A.68}$$

which naturally gives zero for any pair of equal quantum numbers. Note that in general this is an approximation of the real fermionic many-body wave function and it's most commonly used in electronic structure calculations.

Annihilation and Creation Operators

Consider first the case of fermions (antisymmetric WFs). The creation operator $\hat{C}_\alpha^\dagger$ is defined by the relations

$$\hat{C}_\alpha^\dagger|0\rangle = |\alpha\rangle := |\phi_\alpha\rangle; \tag{A.69}$$
$$\hat{C}_\alpha^\dagger|\beta\rangle = \hat{C}_\alpha^\dagger\hat{C}_\beta^\dagger|0\rangle = |\alpha\beta\rangle = -|\beta\alpha\rangle; \tag{A.70}$$
$$\hat{C}_\alpha^\dagger|\beta\gamma\rangle = \hat{C}_\alpha^\dagger\hat{C}_\beta^\dagger\hat{C}_\gamma^\dagger|0\rangle = |\alpha\beta\gamma\rangle, \tag{A.71}$$
$$\text{etc.}$$

The Pauli exclusion principle requires that

$$\hat{C}_\alpha^\dagger|\alpha\cdots\rangle = 0. \tag{A.72}$$

The adjoint operator $\hat{C}_\alpha := \left(\hat{C}_\alpha^\dagger\right)^\dagger$ defines the annihilation operator

$$\hat{C}_\alpha|\alpha\rangle = |0\rangle; \tag{A.73}$$
$$\hat{C}_\alpha|0\rangle = 0. \tag{A.74}$$

It is easy to show (homework) that these fermionic operators obey an *anticommutation* relation

$$\left\{\hat{C}_\alpha, \hat{C}_\beta^\dagger\right\} := \hat{C}_\alpha\hat{C}_\beta^\dagger + \hat{C}_\beta^\dagger\hat{C}_\alpha = \delta_{\alpha\beta}\hat{\mathrm{I}}, \tag{A.75}$$

and the number operator is given by

$$\hat{N} = \sum_\alpha \hat{C}_\alpha^\dagger\hat{C}_\alpha. \tag{A.76}$$

Similarly, for the case of bosons (symmetric WFs) the creation operator $\hat{a}_\alpha^\dagger$ is defined by the relations

$$\hat{a}_\alpha^\dagger|0\rangle = |\phi_\alpha\rangle = |0, 0, \cdots, n_\alpha = 1, 0, \cdots\rangle; \tag{A.77}$$
$$\hat{a}_\alpha^\dagger|n_1, n_2, \cdots, n_\alpha, \cdots\rangle \propto |n_1, n_2, \cdots, n_\alpha + 1, \cdots\rangle, \tag{A.78}$$

and the annihilation operator $\hat{a}_\alpha := \left(\hat{a}_\alpha^\dagger\right)^\dagger$

$$\hat{a}_\alpha|\phi_\alpha\rangle = |0\rangle; \tag{A.79}$$
$$\hat{a}_\alpha|n_1, n_2, \cdots, n_\alpha, \cdots\rangle \propto |n_1, n_2, \cdots, n_\alpha - 1, \cdots\rangle \ (n_\alpha > 0); \tag{A.80}$$
$$\hat{a}_\alpha|n_1, n_2, \cdots, n_\alpha = 0, \cdots\rangle = 0. \tag{A.81}$$

The number operator is given by

$$\hat{N} = \sum_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}, \tag{A.82}$$

and

$$\hat{a}_{\alpha} |n_1, n_2, \cdots, n_{\alpha}, \cdots\rangle = (n_{\alpha})^{\frac{1}{2}} |n_1, n_2, \cdots, n_{\alpha} - 1, \cdots\rangle; \tag{A.83}$$

$$\hat{a}_{\alpha}^{\dagger} |n_1, n_2, \cdots, n_{\alpha}, \cdots\rangle = (n_{\alpha} + 1)^{\frac{1}{2}} |n_1, n_2, \cdots, n_{\alpha} + 1, \cdots\rangle. \tag{A.84}$$

$$\tag{A.85}$$

These were proven for the QHO already. The bosonic operators obey a commutation relation

$$\left[\hat{a}_{\alpha}, \hat{a}_{\beta}^{\dagger}\right] \coloneqq \hat{a}_{\alpha} \hat{a}_{\beta}^{\dagger} - \hat{a}_{\beta}^{\dagger} \hat{a}_{\alpha} = \delta_{\alpha\beta} \hat{\mathrm{I}}. \tag{A.86}$$

References for appendix

[1] M. Möttönen, J. Vartiainen, and J. Pekola. 'Experimental Determination of the Berry Phase in a Superconducting Charge Pump'. In: *Phys. Rev. Lett.* 100 (17 Apr. 2008), p. 177201. DOI: 10.1103/PhysRevLett.100.177201 (cited on page 80).