

PHYS-C0252 - Quantum Mechanics 2022

Lecture notes

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Part I

Mikko's lectures

1.1 Intended learning outcomes

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

1.2 Preface

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

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

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. $\| |\psi_n\rangle - |\psi_m\rangle \| \rightarrow 0$ for $n, m \rightarrow \infty$ then $\exists|\Psi\rangle \in \mathcal{H}$ s.t. $|\psi_m\rangle \rightarrow |\Psi\rangle$ for $m \rightarrow \infty$.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.

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 functional² acting on \mathcal{H} . The so-called Riesz representation theorem³ states that for any linear

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 $u, v, w \in V$, $+: V \times V \rightarrow V$, $a, b \in F$, 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.

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

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

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

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

1.5 Linear operators

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

$$\hat{A}(a|\psi\rangle + b|\phi\rangle) = a\hat{A}|\psi\rangle + b\hat{A}|\phi\rangle. \quad (1.1)$$

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

$$|\hat{A}\psi\rangle := \hat{A}|\psi\rangle := \hat{A}(|\psi\rangle). \quad (1.2)$$

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

$$\hat{A}(\hat{B}|\psi\rangle) = (\hat{A}\hat{B})|\psi\rangle. \quad (1.3)$$

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 $|\psi\rangle\langle\phi| : \mathcal{H} \rightarrow \mathcal{H}$, where $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ s.t. $\forall |\chi\rangle \in \mathcal{H}$ we have:

$$(|\psi\rangle\langle\phi|)|\chi\rangle = |\psi\rangle\langle\phi|\chi\rangle = \langle\phi|\chi\rangle|\psi\rangle \quad (1.4)$$

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

2.1 Intended learning outcomes

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

2.2 Bases of \mathcal{H}

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

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

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

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

1: Defined similarly for infinite-dimensional spaces.

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

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

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

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

$$|\psi\rangle = \sum_k c_k |\phi_k\rangle \quad (2.2)$$

$$\implies \langle \phi_m | \psi \rangle = \sum_k c_k \langle \phi_m | \phi_k \rangle = c_m. \quad (2.3)$$

In other words, we can express the coefficient c_k of the k th 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

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

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

$$\begin{aligned} |\psi\rangle &= \sum_k c_k |\phi_k\rangle \\ &\hat{=} \underbrace{\begin{bmatrix} c_1 \\ 0 \\ 0 \\ \vdots \end{bmatrix}}_{c_1|\phi_1\rangle} + \underbrace{\begin{bmatrix} 0 \\ c_2 \\ 0 \\ \vdots \end{bmatrix}}_{c_2|\phi_2\rangle} + \underbrace{\begin{bmatrix} 0 \\ 0 \\ c_3 \\ \vdots \end{bmatrix}}_{c_3|\phi_3\rangle} + \cdots = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}, \end{aligned} \quad (2.5)$$

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 $|\psi\rangle$:

$$\langle\psi| \hat{=} [c_1^* \quad c_2^* \quad c_3^* \quad \dots]. \quad (2.6)$$

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,

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

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:

$$\hat{A}|\psi\rangle = \sum_{m,k,l} A_{mk} |\phi_m\rangle\langle\phi_k|c_l|\phi_l\rangle \quad (2.8)$$

$$= \sum_{m,k,l} A_{mk}c_l |\phi_m\rangle \underbrace{\langle\phi_k|\phi_l\rangle}_{=\delta_{kl}} \quad (2.9)$$

$$= \sum_{m,k} A_{mk}c_k |\phi_m\rangle.$$

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 Adjugate

Let $\hat{A} \in \mathcal{L}(\mathcal{H})$, and furthermore, let \hat{A} be bounded.² We define the action of \hat{A} on a left-lying bra vector (i.e. an element in the dual

Math on complex conjugation

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

$$z = x + iy$$

$$z^* = x - iy$$

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

space \mathcal{H}^*), $\hat{A} : \mathcal{H}^* \rightarrow \mathcal{H}^*$, $\forall |\phi\rangle, |\psi\rangle \in \mathcal{H}$ through the relation

$$\langle \phi | \hat{A} | \psi \rangle = \langle \phi | (\hat{A} | \psi \rangle). \quad (2.10)$$

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

$$\hat{A}^\dagger |\phi\rangle = |\phi'\rangle, \quad (2.11)$$

which is referred to as the *adjugate* of \hat{A} . The symbol \dagger is pronounced “dagger”, and \hat{A}^\dagger is pronounced “A dagger”.

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 $c \in \mathbb{C}$

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

Thus, $c^\dagger = c^* \in \mathbb{C}$, i.e., the adjugate 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:

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

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

$$\hat{A} |\psi\rangle \hat{=} \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix}. \quad (2.14)$$

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

$$|\phi'\rangle \hat{=} \begin{bmatrix} z \\ w \end{bmatrix} \quad (2.15)$$

that satisfies

$$\langle \phi' | = \langle \phi | \hat{A} \hat{=} [z^* \quad w^*]. \quad (2.16)$$

Using the definition of the inner product, we have³

About notation

These are equivalent:

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

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.

$$\langle \phi | \hat{A} | \psi \rangle = \langle | \phi \rangle, \hat{A} | \psi \rangle \quad (2.17)$$

$$\begin{aligned} &= \left(\begin{bmatrix} x \\ y \end{bmatrix}, \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix} \right) \\ &= \begin{bmatrix} x^* & y^* \end{bmatrix} \begin{bmatrix} au + bv \\ cu + dv \end{bmatrix} \\ &= x^*(au + bv) + y^*(cu + dv). \end{aligned} \quad (2.18)$$

But on the other hand

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

which means that

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

$$\Rightarrow z = (x^*a + y^*c)^* = xa^* + yc^* \quad (2.21)$$

$$w = (x^*b + y^*d)^* = xb^* + yd^*. \quad (2.22)$$

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

$$\hat{A}^\dagger | \phi \rangle = | \phi' \rangle \hat{=} A^\dagger \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} z \\ w \end{bmatrix} = \begin{bmatrix} xa^* + yc^* \\ xb^* + yd^* \end{bmatrix}. \quad (2.23)$$

We can clearly see that this matrix is

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

In other words, the matrix representation of the adjugate \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 adjugate

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

$$(\hat{A}^\dagger)^\dagger = \hat{A}, \quad (2.25)$$

$$(a\hat{A})^\dagger = a^* \hat{A}^\dagger, \quad (a \in \mathbb{C}), \quad (2.26)$$

$$(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger, \quad (2.27)$$

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger, \quad (2.28)$$

$$(|\psi\rangle\langle\phi|)^\dagger = |\phi\rangle\langle\psi|, \quad (2.29)$$

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

$$(\hat{A}|\psi\rangle)^\dagger = \langle\psi|\hat{A}^\dagger. \quad (2.31)$$

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*

$$\hat{A}|\psi_k\rangle = \lambda_k |\psi_k\rangle \quad (2.32)$$

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 $i = 1, \dots, g_k$. The number of eigenvectors g_k corresponding to λ_k is referred to as the *degeneracy* of λ_k .

2.8 Hermitian operators

Definition 2.8.1 The operator $\hat{H} \in \mathcal{L}(\mathcal{H})$ is defined to be Hermitian iff⁴ $\hat{H}^\dagger = \hat{H}$.

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

$$\hat{H} |\psi_k\rangle = \lambda_k |\psi_k\rangle. \quad (2.33)$$

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

$$\hat{H} = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k|. \quad (2.34)$$

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.

2.9 Postulates of quantum mechanics

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

Postulate I

For each physical system there exists a corresponding (rigged)⁵ Hilbert space.

5: We discuss this later

Postulate II

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

Postulate III

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

In an ideal measurement of the quantity A , any measurement outcome equals to an eigenvalue of \hat{A} .⁶

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

$$P(a_n) := \sum_{i=1}^{g_n} |\langle \phi_{n,i} | \psi \rangle|^2. \quad (2.35)$$

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. (2.35), we get the exact same result:

$$\sum_{i=1}^{g_n} |\langle \phi_{n,i} | e^{i\varphi} |\psi\rangle|^2 = \sum_{i=1}^{g_n} \underbrace{|e^{i\varphi}|^2}_{=1} |\langle \phi_{n,i} | \psi \rangle|^2 = P(a_n). \quad (2.36)$$

This is why a global phase offset cannot be measured.

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

$$|\psi'\rangle = \frac{\hat{P}_n |\psi\rangle}{\|\hat{P}_n |\psi\rangle\|}, \quad \hat{P}_n = \sum_{i=1}^{g_n} |\phi_{n,i}\rangle \langle \phi_{n,i}|. \quad (2.37)$$

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

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

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:

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

See the Brief Summary for more details.

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

Postulate VI: Temporal evolution

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

$$i\hbar\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle, \quad (2.38)$$

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.⁷

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.

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

3.1 Intended learning outcomes

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

3.2 Expectation values

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

$$\langle \hat{A} \rangle_\psi = \langle \hat{A} \rangle := \langle \psi | \hat{A} | \psi \rangle. \quad (3.1)$$

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 may be 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

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

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.¹

3.3 Variance

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

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

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

3.4 Continuous bases

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

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

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 possible to normalize. This is why we consider *rigged* Hilbert spaces, which allow such states.²

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

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

1: The theory of probabilistically prepared quantum states is described by the so-called *density matrix formalism*, which is not discussed here.

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

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

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

2: 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.

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

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

Using the definition of the identity operator from Eq. (3.5) above, we can see that the inner product between two vectors $|\phi\rangle$ and $|\chi\rangle$ in a continuous basis is given by

$$\begin{aligned} \langle \phi | \chi \rangle &= \langle \phi | \left(\int |\psi_\alpha\rangle \langle \psi_\alpha| d\alpha \right) | \chi \rangle & (3.6) \\ &= \int \langle \phi | \psi_\alpha \rangle \langle \psi_\alpha | \chi \rangle d\alpha \\ &= \int \phi^*(\alpha) \chi(\alpha) d\alpha, \end{aligned}$$

where $\phi^*(\alpha) := (\phi(\alpha))^*$.

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 $|\psi_x\rangle$).³ The wave function is then a function of position: $\psi(x) := \langle x | \psi \rangle$, and the probability density of finding the particle at x is $|\psi(x)|^2$.

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 $|x\rangle$:

$$\begin{aligned} |\psi\rangle &= \hat{I} |\psi\rangle = \left(\int |x\rangle \langle x| dx \right) |\psi\rangle & (3.7) \\ &= \int |x\rangle \langle x | \psi \rangle dx \\ &= \int |x\rangle \underbrace{\psi(x)}_{\in \mathbb{C}} dx \\ &= \int \psi(x) |x\rangle dx. \end{aligned}$$

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 3.4.1 *In a continuous basis $\{|\psi\rangle_\alpha\}$, the measurement probability of the measurement outcome to reside in the interval*

³: 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 $\vec{x} \in \mathbb{R}^3$.

$[\alpha, \alpha + d\alpha]$ is defined by

$$dP(\alpha) = |\langle \psi_\alpha | \psi \rangle|^2 d\alpha. \quad (3.8)$$

3.5 Commutators

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

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

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

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

3.6 Classical pendulum

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

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

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

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

$$q = l\theta. \quad (3.9)$$

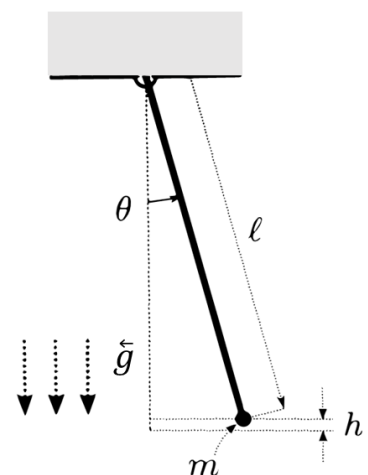


Figure 3.1: Ideal classical pendulum, where a mass m is attached to a massless rigid rod of length l . The rod may rotate without friction about a single axis as described by the angle θ . We assume a uniform gravitational field described by g .

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

$$\begin{aligned} V &= gmh & (3.10) \\ &= mgl(1 - \cos \theta) \approx \frac{1}{2}mgl\theta^2 = \frac{mg}{2l}q^2. \end{aligned}$$

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

$$T = \frac{1}{2}mv^2 = \frac{1}{2}ml^2\dot{\theta}^2 = \frac{1}{2}m\dot{q}^2. \quad (3.11)$$

Definition 3.6.1 *The Lagrangian is defined as*

$$L := T - V. \quad (3.12)$$

Thus, the Lagrangian for our case is

$$\begin{aligned} L &= T - V = \frac{1}{2}ml^2\dot{\theta}^2 - \frac{1}{2}mgl\theta^2 & (3.13) \\ &= \frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2. \end{aligned}$$

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

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

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

$$p = \frac{\partial}{\partial \dot{q}} \left(\frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2 \right) = m\dot{q}. \quad (3.14)$$

Definition 3.6.3 *The classical Hamiltonian is defined as*

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

Using this, we obtain the Hamiltonian of the pendulum (i.e. the

Math on dot notation

$$\dot{y} = \frac{dy}{dt} \neq \frac{\partial y}{\partial t}$$

generally

Math on Taylor series

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

1D harmonic oscillator):

$$\begin{aligned} H = \dot{q}p - L &= m\dot{q}^2 - \left(\frac{1}{2}m\dot{q}^2 - \frac{mg}{2l}q^2 \right) \\ &= \frac{p^2}{2m} + \frac{mg}{2l}q^2 = T + V. \end{aligned} \quad (3.15)$$

3.7 Quantizing a classical system

The term *quantization* 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:

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

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 $[\hat{p}_i, \hat{q}_i] = \hat{p}_i\hat{q}_i - \hat{q}_i\hat{p}_i = -i\hbar$, which is referred to as the *canonical commutation relation* (CCR).
4. **Temporal evolution:** With the above operators and the constraint imposed by the CCR, the temporal evolution of the system is given by the Schrödinger equation $i\hbar\partial_t |\psi\rangle = \hat{H} |\psi\rangle$.

For the pendulum discussed above, the quantization procedure simply yields

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mg}{2l}\hat{q}^2. \quad (3.16)$$

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

The above procedure maybe used for many different systems. For example, it is possible to quantize electric circuits by choosing charge as the generalized position and magnetic flux as the momentum, or vice versa.⁴ Another important application is the quantization of the electromagnetic field, which follows a similar procedure but with a continuous set of generalized coordinates.

4: This is discussed in the Quantum Circuits course.

4.1 Intended learning outcomes

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

4.2 One-dimensional quantum harmonic oscillator

As we derived above in Eq. (3.16), the operator corresponding to the classical Hamiltonian of the harmonic oscillator is given by

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

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

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

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

$$\hat{H} = (A\hat{q} - iB\hat{p})(A\hat{q} + iB\hat{p}) + C. \quad (4.3)$$

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

$$\begin{aligned} \hat{H} &= A^2 \hat{q}^2 + iAB\hat{q}\hat{p} - iB\hat{p}A\hat{q} + B^2 \hat{p}^2 + C & (4.4) \\ &= A^2 \hat{q}^2 + B^2 \hat{p}^2 + \underbrace{iAB [\hat{q}, \hat{p}]}_{=i\hbar} + C. \\ & & \underbrace{\hspace{1.5cm}}_{=-\hbar AB} \end{aligned}$$

Math on \mathbb{C}

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

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

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

Comparing this to Eq. (4.2), we choose

$$A = \sqrt{\frac{1}{2}m\omega^2}, \quad (4.5)$$

$$B = \sqrt{\frac{1}{2m}}, \quad (4.6)$$

$$C = \hbar AB = \frac{\hbar\omega}{2}. \quad (4.7)$$

With these, we may write

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

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

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

from which it follows that

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

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

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

Some observations about the quantum harmonic oscillator:

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

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

Thus all eigenenergies are positive.

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

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

In other words, $|\psi'\rangle = \hat{a} |\psi\rangle$ is also an eigenstate of \hat{H} , with energy $\varepsilon - \hbar\omega$. Similarly, we have $\hat{H} \hat{a}^\dagger |\psi\rangle = (\varepsilon + \hbar\omega) \hat{a}^\dagger |\psi\rangle$. 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 $|0\rangle$:

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

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

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

4.3 Symbolic operator differential

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

Such a conjugate pair satisfies the commutation relation $[\hat{q}, \hat{p}] = i\hbar$. Some calculations are simplified if we symbolically define $\hat{p} = -i\hbar\partial_{\hat{q}}$, 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, $\forall |\psi\rangle \in \mathcal{H}$

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

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

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

$$\begin{aligned} [\hat{q}, \hat{p}] &= \hat{q}\hat{p} - \hat{p}\hat{q} & (4.14) \\ &= \hat{q}(-i\hbar\partial_{\hat{q}}) - (-i\hbar\partial_{\hat{q}})\hat{q} \\ &= -i\hbar\hat{q}\partial_{\hat{q}} + i\hbar\partial_{\hat{q}}\hat{q} \\ &= -i\hbar\hat{q}\partial_{\hat{q}} + i\hbar \underbrace{(\partial_{\hat{q}}\hat{q})}_{=1} + i\hbar\hat{q}\partial_{\hat{q}} \\ &= i\hbar. \end{aligned}$$

4.4 Solving the ground state in the position representation

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

$$\begin{aligned} 0 &= \langle x' | \hat{a} | 0 \rangle & (4.15) \\ &= \langle x' | \underbrace{\sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + \frac{i}{m\omega} (-i\hbar\partial_{\hat{x}}) \right)}_{=\hat{a}} \underbrace{\left(\int d\tilde{x} |\tilde{x}\rangle \langle \tilde{x}| \right)}_{=\hat{1}} | 0 \rangle \\ &= \sqrt{\frac{m\omega}{2\hbar}} \int d\tilde{x} \underbrace{\langle x' | \tilde{x} \rangle}_{\delta(\tilde{x}-x')} \left(\tilde{x} + \frac{\hbar}{m\omega} \partial_{\tilde{x}} \right) \underbrace{\psi_0(\tilde{x})}_{=:\langle \tilde{x} | 0 \rangle} \end{aligned}$$

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

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

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

We may further derive the wave function of the first excited state from $\psi_1(x) = \langle x|1\rangle = \tilde{C} \langle x| \hat{a}^\dagger |0\rangle$ where we do not even need to solve a differential equation since we know $\psi_0(x)$ and we may simply multiply it and take the first derivative. Similarly, we may proceed to derive the wave function of any state $|n\rangle$. However, we do not do this here, but come back to the harmonic oscillator on the second half of the course where we study the wave functions of the excited states further.

4.5 Uncertainty relations

Definition 4.5.1 *The Heisenberg uncertainty relation is defined as*

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

where $\Delta A^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$ and $[\hat{q}, \hat{p}] = i\hbar$ since \hat{q} and \hat{p} are a canonical conjugate pair¹.

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

Definition 4.5.2 *The Robertson uncertainty relation is defined as*

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

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

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

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

and similarly,

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

Math on norm of C

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

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

Then, the Cauchy-Schwarz inequality implies

$$|\langle f|g\rangle| \leq \|f\| \|g\| \quad (4.22)$$

$$\Rightarrow \Delta A^2 \Delta B^2 \geq \underbrace{|\langle f|g\rangle|^2}_{\in \mathbb{C}} \quad (4.23)$$

$$\begin{aligned} &= |\langle \psi | (\hat{A} - \langle \hat{A} \rangle \hat{I}) (\hat{B} - \langle \hat{B} \rangle \hat{I}) | \psi \rangle|^2 \\ &\geq \frac{|\langle \psi | (\hat{A} - \langle \hat{A} \rangle \hat{I}) (\hat{B} - \langle \hat{B} \rangle \hat{I}) | \psi \rangle - \langle \psi | (\hat{B} - \langle \hat{B} \rangle \hat{I}) (\hat{A} - \langle \hat{A} \rangle \hat{I}) | \psi \rangle|^2}{4} \\ &= \frac{|\langle \psi | [\hat{A} - \langle \hat{A} \rangle \hat{I}, \hat{B} - \langle \hat{B} \rangle \hat{I}] | \psi \rangle|^2}{4} \\ &= \frac{|\langle [\hat{A}, \hat{B}] \rangle|^2}{4} \quad \square \end{aligned}$$

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:

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

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

$$e^{\hat{A}} := \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}. \quad (5.2)$$

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

With this definition,

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

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

Math on a diff.eq.

$$\partial_x f(x) = \lambda f(x) \implies f(x) = Ae^{\lambda x}$$

The temporal evolution can then be written as

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

where $\hat{U}(t) = \exp(-i\hat{H}t/\hbar)$ 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

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

from which it follows that

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

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

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

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

5.3 Case of temporally dependent Hamiltonian

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

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

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

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

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

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

This is equivalent to the Schrödinger equation.

Exercise

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

5.4 Properties of unitary operators

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

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

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

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

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

for which we have

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

Unitary operators can be considered as rotations.²

2: sometimes reflections as well

5.5 Qubit

A qubit can refer either to a physical system or to a mathematical construction. In either case, it is modeled by a 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

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

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

Thus,

$$\begin{aligned} \hat{H}_q &= \varepsilon_1 |g\rangle\langle g| + \varepsilon_2 |e\rangle\langle e| \tag{5.16} \\ &= \frac{\varepsilon}{2} (-|g\rangle\langle g| + |e\rangle\langle e|) + \frac{(\varepsilon_1 + \varepsilon_2)}{2} |g\rangle\langle g| + \frac{(\varepsilon_1 + \varepsilon_2)}{2} |e\rangle\langle e| \\ &= \frac{\varepsilon}{2} (-|g\rangle\langle g| + |e\rangle\langle e|) + \underbrace{\frac{\varepsilon_1 + \varepsilon_2}{2} \hat{I}} \end{aligned}$$

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

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

Thus,

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

The temporal evolution is given by

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

5.6 How to set up a qubit from a physical system

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

3: Ground and excited

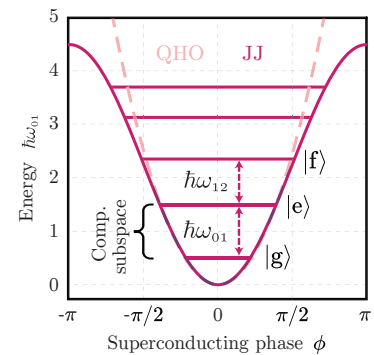


Figure 5.1: Non-linear harmonic oscillator with a Josephson junction (JJ). Notice that the gap $\hbar\omega_{01} \neq \hbar\omega_{12}$, i.e., the energy states are non-equidistant. Figure from Ref. [1].

5.7 Pauli operators

Definition 5.7.1 The Pauli operators are

$$\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \quad (5.19)$$

$$\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \quad (5.20)$$

$$\hat{\sigma}_y = -i|0\rangle\langle 1| + i|1\rangle\langle 0| \quad (5.21)$$

Properties

The Pauli operators have a number of interesting properties:

$$\hat{\sigma}_\alpha^2 = \hat{I} \quad \forall \alpha \in \{x, y, z\} \quad (5.22)$$

$$\hat{\sigma}_\alpha^\dagger = \hat{\sigma}_\alpha \quad \forall \alpha \quad (5.23)$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = \sum_{k \in \{x, y, z\}} 2i\hat{\sigma}_k \varepsilon_{ijk}, \quad \forall i, j \in \{x, y, z\}, \quad (5.24)$$

where

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

is the Levi-Civita symbol.

Definition 5.7.2

$$\hat{\sigma}^- = |0\rangle\langle 1| \quad (5.26)$$

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

Exercise

Show that

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

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

5.8 Bloch sphere

Definition 5.8.1 A qubit state can always be expressed as

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

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

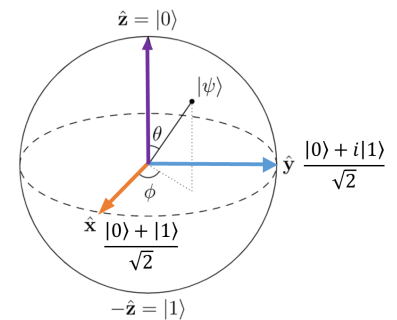


Figure 5.2: Bloch sphere representation [2].

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

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

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

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

Exercise

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

Last lecture from Mikko.

6.1 Intended learning outcomes

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

6.2 Tunable Hamiltonian for quantum gates

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

Thus any unitary evolution¹ $\hat{U} = \hat{I} \cos \theta + i \vec{b} \cdot \hat{\sigma} \sin \theta$ can be implemented, for example, by a control sequence

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

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

$$\hat{H} = -\frac{\varepsilon}{2} \hat{\sigma}_z \quad (6.2)$$

and apply a field $\vec{H}_{\text{ex}}(t) = \frac{\Omega}{2} \hat{\sigma}_x \sin(\omega t + \phi)$, 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 $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \hat{=} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.
- ▶ Hadamard gate corresponds to $\hat{H}_g = \frac{1}{\sqrt{2}} (\hat{\sigma}_x + \hat{\sigma}_z) \hat{=} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$.
- ▶ Phase flip corresponds to $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \hat{=} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.

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

Exercise

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

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

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

$$P_0 = |\langle 0|\psi\rangle|^2 = |c_0|^2 \quad (6.3)$$

$$P_1 = |\langle 1|\psi\rangle|^2 = |c_1|^2 = 1 - |c_0|^2 \quad (6.4)$$

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

$$P_0 = |\langle 0|\hat{U}|\psi\rangle|^2 = \langle \psi|\hat{U}^\dagger|0\rangle\langle 0|\hat{U}|\psi\rangle = |\langle \tilde{0}|\psi\rangle|^2, \quad (6.5)$$

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

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 $\hat{A}_2 \in \mathcal{L}(\mathcal{H}_2^{(2)})$.

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

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

On the tensor product

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

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

$$|00\rangle := |0\rangle \otimes |0\rangle \quad (6.7)$$

$$|01\rangle := |0\rangle \otimes |1\rangle \quad (6.8)$$

$$|10\rangle := |1\rangle \otimes |0\rangle \quad (6.9)$$

$$|11\rangle := |1\rangle \otimes |1\rangle, \quad (6.10)$$

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

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

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

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

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

6.6 Examples of two-qubit gates

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

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

Exercise

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

6.7 n -qubit system

For a system with n qubits, we usually define $N := 2^n = \dim \{\mathcal{H}_2^n\}$, and we have the following properties:

- ▶ $\mathcal{H}_{2^n} = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)} \otimes \dots \otimes \mathcal{H}_2^{(n)}$
- ▶ $|\psi\rangle = \sum_{k=0}^{2^n-1} c_k |k\rangle = c_0 \underbrace{|00\dots 0\rangle}_{n \text{ zeroes}} + c_1 \underbrace{|0\dots 01\rangle}_{n-1 \text{ zeroes}} + \dots$, where again $|k\rangle$ means $|k_1 k_2 \dots k_n\rangle$, where $k_1 k_2 \dots k_n$ is k written in binary
- ▶ $\underbrace{\hat{I} \otimes \dots \otimes \hat{I}}_{m-1} \otimes \hat{A} \otimes \underbrace{\hat{I} \otimes \dots \otimes \hat{I}}_{n-m}$ 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. \rightarrow 4. and initializes and measures all qubits in 1. and 3., respectively.

Exercise

Deutsch 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.

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \quad (6.14)$$

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

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

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

6.10 Commuting operators

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

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

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

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

References

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- [2] Wikimedia Commons. *File:Bloch Sphere.svg* — *Wikimedia Commons, the free media repository*. [Online; accessed 5th August 2021]. 2020. URL: https://commons.wikimedia.org/w/index.php?title=File:Bloch_Sphere.svg&oldid=514662857 (cited on page 30).

Part II

Tapio's lectures

This lecture presents a more detailed treatment of the quantum harmonic oscillator introduced in Lecture 4. In particular, we discuss the nature of the actual real-space wave functions and their physical meaning. 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.

7.1 Intended learning outcomes

- ▶ Deepen knowledge on harmonic oscillators and their applications
- ▶ Learn how to apply and manipulate the raising and lowering operators with number states
- ▶ Understand the nature of the eigenfunctions in real space

7.2 Classical Harmonic Oscillators

Harmonic oscillators appear in many applications in classical and quantum physics (photons, lattice vibrations i.e. phonons, etc.). They have turned out to be most important for describing open quantum systems interacting with a large environment (called the "heat bath"), which is often modeled by a set of quantum harmonic oscillators (QHOs).

For mutually interacting atoms in a classical solid lattice we can write the general (classical) Hamiltonian as

$$H = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + V(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N), \quad (7.1)$$

where \vec{p}_i and \vec{r}_i are the momentum and position of atom i , respectively, m is the mass of a atom (same for all atoms), and V is a potential function describing the interaction between the atoms.

For small displacements $\vec{u}_i = \vec{r}_i - \vec{R}_i$ around the fixed equilibrium positions \vec{R}_i , the interaction potential can be expanded in Taylor

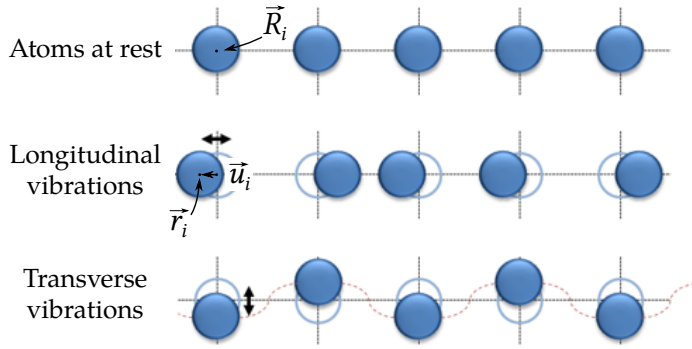


Figure 7.1: Atoms vibrating around the equilibrium lattice positions \vec{R}_i in a 1D lattice.

series as

$$V \approx V_0 \sum_{i,j} \underbrace{\frac{\partial V^j}{\partial x_i}}_{=0} u_{x_{ij}} + \frac{1}{2} \sum_{i,j,k,l} \frac{\partial^2 V^{kl}}{\partial x_i \partial x_j} u_{x_{ik}} u_{x_{jl}}, \quad (7.2)$$

which is called the *Harmonic Approximation*. Note that the first term on the l.h.s. of the equation is force that has to vanish in equilibrium (mechanical balance). The classical pendulum of Section 3.6 is an example of this expansion (cf. Eq. (3.16)). By diagonalizing (in normal coordinates) the classical harmonic Hamiltonian can be written as

$$H(q_1, \dots, q_N, p_1, \dots, p_N) = \sum_{i=1}^{3N} \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 q_i^2, \quad (7.3)$$

for identical but distinguishable particles in 3D space.

The equations of motion can be obtained from the standard Hamilton equations as

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}; \quad (7.4)$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}. \quad (7.5)$$

The equations of motion are linear and can be easily solved (1D homework problem).

7.3 Quantum Harmonic Oscillators

Consider a single 1D Quantum Harmonic Oscillator (QHO) whose Hamiltonian is given by (see Section 4.2)

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{q}^2, \quad (7.6)$$

which we have obtained by simple quantization from the classical Hamiltonian as $x \rightarrow \hat{q}$, $p \rightarrow \hat{p}$ where

$$[\hat{q}, \hat{p}] = i\hbar. \quad (7.7)$$

Next it is useful to define dimensionless operators as

$$\hat{Q} := \sqrt{\frac{m\omega}{\hbar}} \hat{q}; \quad (7.8)$$

$$\hat{P} := \sqrt{\frac{1}{m\hbar\omega}} \hat{p}, \quad (7.9)$$

which now satisfy $[\hat{Q}, \hat{P}] = i$. This gives us the Hamiltonian

$$\hat{H} = \frac{1}{2} \hbar\omega (\hat{P}^2 + \hat{Q}^2). \quad (7.10)$$

The next trick is to introduce two new operators that are Hermitian conjugates as

$$\hat{a} = \frac{\hat{Q} + i\hat{P}}{\sqrt{2}}; \quad (7.11)$$

$$\hat{a}^\dagger = \frac{\hat{Q} - i\hat{P}}{\sqrt{2}}, \quad (7.12)$$

that now satisfy

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (7.13)$$

The 1D QHO Hamiltonian can now be written as

$$\hat{H} = \frac{1}{2} \hbar\omega (\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}) \quad (7.14)$$

$$= \hbar\omega \left(\hat{a}\hat{a}^\dagger - \frac{1}{2} \right) = \hbar\omega \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right). \quad (7.15)$$

Note that no matter how you write this, it has to be Hermitian (make sure you understand why). The importance of this form is that it allows us to obtain a fully algebraic solution for the QHO without having to explicitly solve for the Schrödinger equation. In this section we will next generalize and extend the treatment in Section 4 of the lecture notes.

The formal (eigen)solution is given by

$$\hbar\omega \left(\hat{a}^\dagger\hat{a} + \frac{1}{2} \right) |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle, \quad (7.16)$$

where n is the eigenvalue of the operator $\hat{a}^\dagger\hat{a}$ corresponding to

eigenstate $|n\rangle$ of the following *number operator*:

$$\hat{N} := \hat{a}^\dagger \hat{a}. \quad (7.17)$$

The number operator satisfies (homework)

$$[\hat{N}, \hat{a}] = -\hat{a}, \quad [\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger. \quad (7.18)$$

Let us assume that \hat{N} has a complete set of orthogonal eigenvectors, *i.e.*, $\hat{N}|n\rangle = n|n\rangle$ (why does this have to be true?). Then it follows that

$$\hat{N}\hat{a}|n\rangle = \hat{a}(\hat{N} - 1)|n\rangle = (n - 1)\hat{a}|n\rangle. \quad (7.19)$$

Similarly

$$\hat{N}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(\hat{N} + 1)|n\rangle = (n + 1)\hat{a}^\dagger|n\rangle. \quad (7.20)$$

It was shown in Chapter 4 that the eigenvalues must be non-negative and the spectrum is bounded from below by the ground state for which $n = 0$.

The two equations above imply that $\hat{a}|n\rangle \propto |n - 1\rangle$ and $\hat{a}^\dagger|n\rangle \propto |n + 1\rangle$. The corresponding proportionality coefficient for the raising operator can be computed from the squared norm of $\hat{a}^\dagger|n\rangle$ as

$$\langle n|\hat{a}(\hat{a}^\dagger|n\rangle) = \langle n|(\hat{N} + 1)|n\rangle = (n + 1)\langle n|n\rangle, \quad (7.21)$$

and thus the amplitude is $\sqrt{n + 1}$, which gives

$$\hat{a}^\dagger|n\rangle = \sqrt{n + 1}|n + 1\rangle. \quad (7.22)$$

Similarly, we can compute that

$$\hat{a}|n\rangle = \sqrt{n}|n - 1\rangle. \quad (7.23)$$

Thus any eigenstate $|n\rangle$ can be written as (prove, *e.g.*, by induction)

$$|n\rangle = (n!)^{-\frac{1}{2}} (\hat{a}^\dagger)^n |0\rangle. \quad (7.24)$$

Another important result is that the elements of the matrix representation of \hat{a}^\dagger and \hat{a} have a simple form:

$$\langle n'|\hat{a}^\dagger|n\rangle = \sqrt{n + 1} \delta_{n',n+1}; \quad (7.25)$$

$$\langle n'|\hat{a}|n\rangle = \sqrt{n} \delta_{n',n-1}, \quad (7.26)$$

where $\delta_{i,j}$ is the Kronecker delta according to Eq. (2.1). Finally, we

can read off the eigenvalues of the Hamiltonian trivially as

$$\hat{H} |n\rangle := E_n |n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle. \quad (7.27)$$

in accordance with the results of Section 4.2.

7.4 Quantum harmonic oscillator in the position basis

The algebraic solution discussed above is mathematically very elegant and convenient: it is simple to manipulate and has a simple solution. However, it is somewhat difficult to grasp how it is physically related to the harmonic oscillator. Here we introduce another way of solving for the eigenfunctions and -values of the QHO, based on writing the Schrödinger equation in its natural coordinate basis. We define the *wave function* as $\psi(x) := \langle x|\psi\rangle$. This is a coordinate representation by using the basis set $\{|x\rangle\}$ of the position operator \hat{x} . Consequently, the time-independent Schrödinger (energy-eigenvalue) equation $\hat{H}\psi = E\psi$ for a single QHO becomes

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \frac{m\omega^2}{2} x^2 \psi(x) = E\psi(x). \quad (7.28)$$

To simplify the equation, it is useful to define

$$q = \sqrt{\frac{m\omega}{\hbar}} x, \quad \lambda = \frac{2E}{\hbar\omega}, \quad \psi(x) = u\left(\sqrt{m\omega/\hbar} x\right) = u(q), \quad (7.29)$$

which gives (check)

$$\frac{d^2 u}{dq^2} + (\lambda - q^2) u = 0. \quad (7.30)$$

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

$$u(q) = H(q)e^{-q^2/2}, \quad (7.31)$$

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

$$H'' - 2qH' + (\lambda - 1)H = 0. \quad (7.32)$$

The solutions of Eq. (7.32) 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. (7.32). Matching terms with equal powers in

the expansion inserted in Eq. (7.32) requires that $\lambda = 2n + 1$ with n being an integer, which gives

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right). \tag{7.33}$$

The Hermite polynomials can be generated through

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}. \tag{7.34}$$

The complete, normalized eigenfunctions of the QHO are given by

$$\psi_n(x) = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right) H_n(\alpha x) e^{-\alpha^2 x^2 / 2}, \tag{7.35}$$

where $\alpha = \sqrt{m\omega/\hbar}$. The eigenfunctions are shown in Fig. 7.2. Fig. 7.3 further demonstrates the potential energy and the probability density for finding the particle at a given point. In the figures, $\xi = q = \alpha x$.

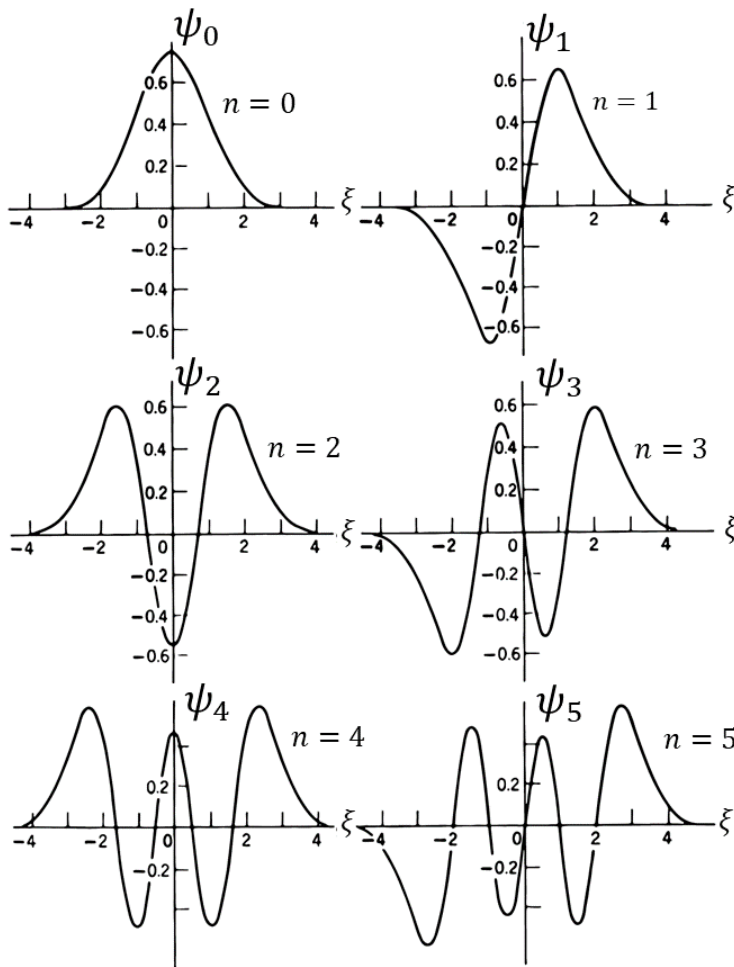


Figure 7.2: Eigenfunctions of the QHO, from Eq. (7.35).

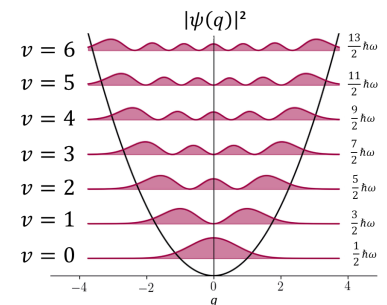


Figure 7.3: Probability (density) of finding a particle in a quadratic potential well at any given point.

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

$$\int_{-\infty}^{\infty} H_n(\xi)H_k(\xi)e^{-\xi^2}d\xi = 0, \quad \text{for } n \neq k. \quad (7.36)$$

The actual (true) inner product between the full wave functions that form a complete orthonormal set is given by (cf. Lecture 1)

$$(\psi_n, \psi_k) \equiv \int_{-\infty}^{\infty} dx \psi_n^*(x)\psi_k(x) = \delta_{nk} \quad (7.37)$$

where in its full form

$$\psi_n(x) = 2^{-\frac{n}{2}}(n!)^{-\frac{1}{2}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega x^2}{2\hbar}\right)H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right). \quad (7.38)$$

This lecture deals with a quantum particle (wave) 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 position basis by explicitly solving for the corresponding Schrödinger equation with proper boundary conditions. We start by revisiting the case of a free particle and highlighting the choice of different basis (position or momentum here), and then discuss the influence of external potentials. Of particular interest are the differences between pointlike classical particles and quantum ones (waves) in external potentials.

8.1 Intended learning outcomes

- ▶ Explain details of plane waves (particles propagating in free space) in different representations
- ▶ Understand the superposition principle for time dependence of the states
- ▶ Learn to solve the Schrödinger equation in simple potential landscapes and understand their influence on the eigenstates, including scattering

8.2 Free Particles and Plane Waves

Consider a free particle that does not experience any external potential (forces) in space. In such a case we can use the symbolic state representation as long as we are not interested in the details of the particle position or momentum. We first (re)define the position and momentum (right) eigenvectors as

$$\hat{x}|x\rangle = x|x\rangle; \quad \hat{p}|p\rangle = p|p\rangle, \quad (8.1)$$

and correspondingly the left eigenvectors

$$\langle x|\hat{x} = \langle x|x; \quad \langle p|\hat{p}^\dagger = \langle p|p. \quad (8.2)$$

The left and right eigenvectors are orthonormal:

$$\langle x'|x\rangle = \delta(x' - x); \quad \langle p'|p\rangle = \delta(p' - p), \quad (8.3)$$

and they form complete orthonormal sets that can be inserted between any states when necessary:

$$\int dx |x\rangle\langle x| = 1; \quad \int dp |p\rangle\langle p| = 1. \quad (8.4)$$

Now we can define the *momentum operator* in the *position basis* as (not derived here)

$$\langle x'|\hat{p}|x\rangle = -i\hbar \delta(x' - x) \frac{d}{dx}. \quad (8.5)$$

The importance of this formula is that this is exactly where the mathematical form of the momentum operator \hat{p} comes from in the (energy-eigenvalue) SE when it's written in the position basis.

Furthermore, we can define the *position operator* in the *momentum basis* as

$$\langle p'|\hat{x}|p\rangle = -i\hbar \delta(p' - p) \frac{d}{dp}. \quad (8.6)$$

Now we can solve for the *momentum eigenstate* in the *position basis* $\psi_p(x) = \langle x|p\rangle$ from the DE

$$\langle x|\hat{p}|p\rangle = -i\hbar \frac{d}{dx} \langle x|p\rangle = p \langle x|p\rangle. \quad (8.7)$$

This equation comes about from the fact that

$$\langle x|\hat{p}|p\rangle = \int dx' \langle x|\hat{p}|x'\rangle \langle x'|p\rangle = \int dx' -i\hbar \delta(x - x') \frac{d}{dx'} \langle x'|p\rangle \quad (8.8)$$

$$= -i\hbar \frac{d}{dx} \langle x|p\rangle. \quad (8.9)$$

Thus we have the differential equation

$$-i\hbar \frac{d}{dx} \langle x|p\rangle = p \langle x|p\rangle. \quad (8.10)$$

The solution to this DE is called a (simple) plane wave

$$\langle x|p\rangle = \sqrt{\frac{1}{2\pi\hbar}} e^{ipx/\hbar}. \quad (8.11)$$

The corresponding *momentum eigenstate* in the *momentum basis* is

$$\psi_p(p') = \langle p'|p\rangle = \delta(p - p'). \quad (8.12)$$

The normalized *position eigenstate* in the *momentum basis* can be

obtained from

$$\langle p|x\rangle = \langle x|p\rangle^\dagger = \sqrt{\frac{1}{2\pi\hbar}} e^{-ipx/\hbar}, \quad (8.13)$$

and the normalized *position eigenstate in the position basis* is (of course)

$$\psi_x(x) = \langle x'|x\rangle = \delta(x - x'). \quad (8.14)$$

Note that these results can also be derived from the free-particle stationary Schrödinger equation. For a free particle, the Hamiltonian operator is $\hat{H} = \hat{p}^2/(2m)$ (which is the same as the Hamiltonian of the quantum harmonic oscillator with zero potential). In the position basis, the stationary Schrödinger equation then reads

$$\hat{H}|\psi\rangle = E|\psi\rangle; \quad (8.15)$$

$$\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x). \quad (8.16)$$

The above position-basis results are the solution of this differential equation.

Time Dependence of Plane Waves

Let us next look at the time 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 is

$$i\hbar \frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x,t)}{dx^2}. \quad (8.17)$$

We look for separable solutions of the form

$$\Psi(x,t) = f(t)\psi(x). \quad (8.18)$$

This gives

$$\frac{i\hbar}{f(t)} \frac{\partial f(t)}{\partial t} = -\frac{1}{\psi(x)} \frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2}. \quad (8.19)$$

Both sides must be constant (why?) and thus

$$f(t) = e^{-iEt/\hbar}, \quad (8.20)$$

where we have already adopted the notation E for the constant because it has to have units of energy (to make the argument in the exponential function dimensionless). Using the plane wave from Eq. (8.11), the time evolution of a plane wave in the position basis

is thus given by

$$\Psi(x, t) = e^{-iEt/\hbar} \langle x|p \rangle = \sqrt{\frac{1}{2\pi\hbar}} e^{-iEt/\hbar} e^{ipx/\hbar}, \quad (8.21)$$

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

$$\partial_t |\Psi(x, t)|^2 = 0. \quad (8.22)$$

For a general state that is a superposition of plane waves with coefficients c_E for each wave with energy E at time $t = 0$,

$$\Psi(x, 0) = \sum_E c_E e^{ipx/\hbar}, \quad (8.23)$$

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

$$\Psi(x, t) = \sum_E c_E e^{-iEt/\hbar} e^{ipx/\hbar}. \quad (8.24)$$

An important generalization of this is that if we use the completeness of the energy eigenfunctions $\psi_E(x)$ to expand in terms of them, then in general it holds that for a state

$$\Psi(x, 0) = \sum_E c_E \psi_E(x) \quad (8.25)$$

the time dependence is given by

$$\Psi(x, t) = \sum_E c_E e^{-iEt/\hbar} \psi_E(x). \quad (8.26)$$

Equivalently, for a continuous energy spectrum, where the coefficients c_E are now a continuous function $c(E)$ of energy,

$$\Psi(x, 0) = \int c(E) \psi_E(x) dE, \quad (8.27)$$

the time evolution is given by

$$\Psi(x, t) = \int c(E) \psi_E(x) e^{-iEt/\hbar} dE. \quad (8.28)$$

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

Particle in a Periodic Box

There is a mathematical subtlety associated with plane waves because they live in an infinite domain and are not normalizable

(why is this the case?). A simple solution to this is to consider a free particle that traverses a box of finite (linear) size L , but no external $V(x)$ (periodic boundary conditions) s.t. $\psi_p(x) = \psi_p(x+L)$. The solution is that of a free particle, but now the momentum is quantized and can be written in terms of the wave number k_n as

$$p_n = \hbar k_n = \frac{2\hbar\pi n}{L}, \quad n \in \mathbb{Z}. \quad (8.29)$$

The completeness relations now read as

$$\int_0^L dx |x\rangle\langle x| = 1; \quad \sum_{n=-\infty}^{\infty} |p\rangle\langle p| = 1. \quad (8.30)$$

The wavevector eigenstate in the **position basis** is then simply

$$\psi_k(x) = \langle x|k\rangle = \langle k|x\rangle^\dagger = \frac{1}{\sqrt{L}} e^{ikx}. \quad (8.31)$$

8.3 Particles in External Potentials

Infinite Potential Well

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

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq a; \\ \infty, & \text{otherwise.} \end{cases} \quad (8.32)$$

Since there is no potential in the well, the solution of the energy-eigenvalue (static) SE there is that of a free particle:

$$\psi''(x) = -k^2\psi(x); \quad k = \frac{\sqrt{2mE}}{\hbar}. \quad (8.33)$$

This is a classical harmonic oscillator, whose solutions are simple sine and cosine waves

$$\psi(x) = A \sin kx + B \cos kx. \quad (8.34)$$

Because the potential is infinite outside of the well, the wave function must be zero there. Symmetry requires that $\psi(0) = \psi(a)$ and thus $B = 0$, and because the function must be zero at boundaries

$$\psi(x) = A \sin kx; \quad ka = 0, \pm\pi, \pm2\pi, \dots, \quad (8.35)$$

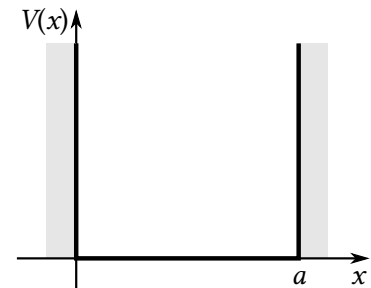


Figure 8.1: Infinite potential well.

i.e., $k_n = n\pi/a$ for $n \in \mathbb{Z}$ which means that the energy is quantized as

$$E_n = \frac{\hbar^2 k_n^2}{2m}. \quad (8.36)$$

Normalization of the wave function gives

$$A = \sqrt{\frac{2}{a}}, \quad (8.37)$$

resulting in

$$\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}, \quad n \in \mathbb{Z}. \quad (8.38)$$

Eq. (8.38) is plotted for the first three values of n in Fig. 8.2.

The stationary states of the time-dependent SE can be obtained from the superposition principle in the energy basis:

$$\Psi_n(x, t) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} e^{-iE_n t/\hbar}. \quad (8.39)$$

Then the most general solution to the time-dependent SE can be written as

$$\Psi(x, t) = \sum_{n=0}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} e^{-iE_n t/\hbar}, \quad (8.40)$$

where the expansion coefficients, c_n , depend on the initial state $\Psi(x, 0)$.

Square-Well Potential

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

$$V(x) = \begin{cases} \infty, & \text{if } -\infty \leq x \leq 0; \\ -V_0, & \text{if } 0 \leq x \leq a, \\ 0, & \text{if } a \leq x \leq \infty. \end{cases} \quad (8.41)$$

It turns out that there are now two types of solutions: *bound* states whose energy is below zero level of the potential and *unbound* (free) states.

First we note that for $x < 0$, $\psi(x) = 0$ as in the previous subsection because the potential is infinitely strong on the l.h.s. For bound

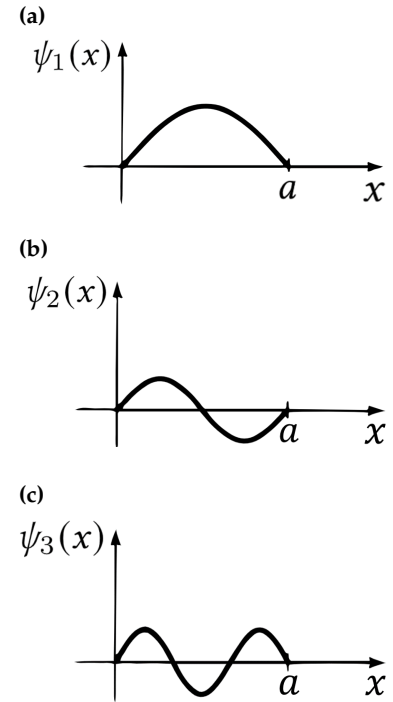


Figure 8.2: Wave function Eq. (8.38) for the modes (a) $n = 1$, (b) $n = 2$, (c) $n = 3$.

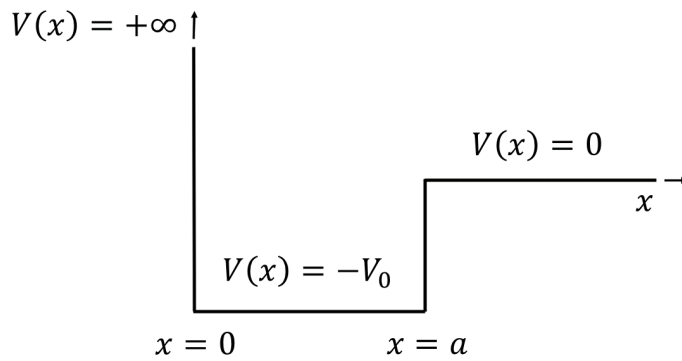


Figure 8.3: Square-well potential.

states, $0 < x < a$,

$$\psi''(x) = -k_0^2 \psi(x); \quad E = \frac{\hbar^2 k_0^2}{2m} - V_0, \quad (8.42)$$

whose (continuous) solution is $\psi(x) = C \sin k_0 x$. This is formally the same as in the infinite-well case, but now the momentum (wave vector) is modified by the potential.

In the third region, $x > a$, the free-particle solution applies (but with negative energy):

$$\psi''(x) = k^2 \psi(x); \quad k^2 = -\frac{2mE}{\hbar^2}. \quad (8.43)$$

Now the general solution is $\psi(x) = Ae^{-kx} + Be^{kx}$, where $B = 0$ (why?).

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

$$k_0 \cot k_0 a = -k^2. \quad (8.44)$$

Because both variables depend on the energy, they have to satisfy

$$k^2 + k_0^2 = \frac{2V_0 m}{\hbar^2}. \quad (8.45)$$

For solutions (**bound** states) to exist, these two equations have to match, see Fig. 8.4.

For the **unbound** states, the wave function is again zero for $x < 0$. For $0 < x < a$, the bound state equation turns into

$$\psi''(x) = -k_0^2 \psi(x); \quad E = \frac{\hbar^2 k_0^2}{2m} - V_0, \quad (8.46)$$

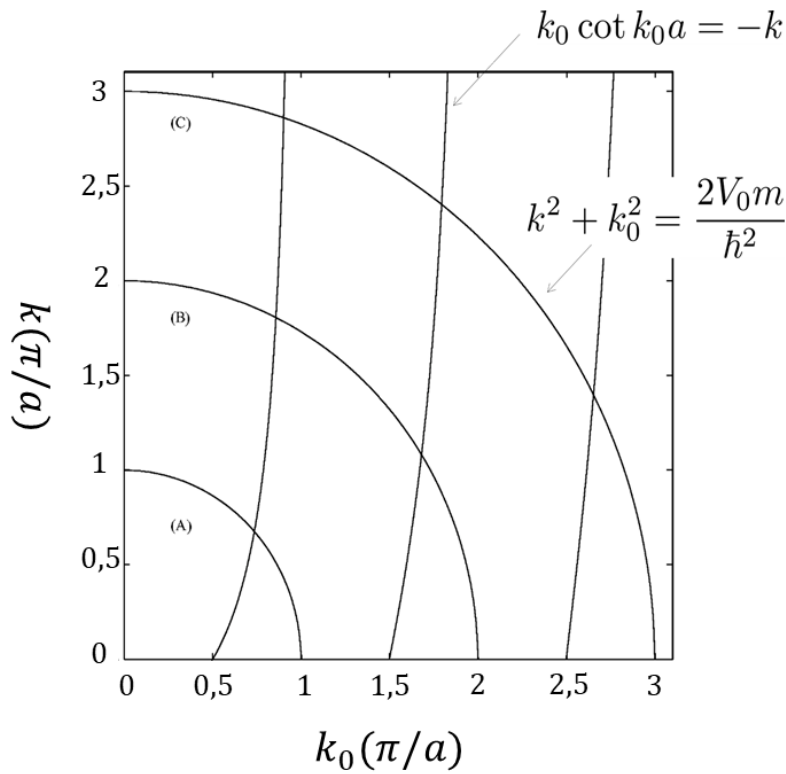


Figure 8.4: Allowed parameters for bound states.

with the solution $\psi(x) = C \sin k_0 x$. In the last region, $a < x < \infty$,

$$\psi''(x) = -k^2 \psi(x); \quad E = \frac{\hbar^2 k^2}{2m}, \quad (8.47)$$

and we need to include the phase shift

$$\psi(x) = D \sin(kx + \delta). \quad (8.48)$$

The continuity condition at a now gives

$$k_0 \cot k_0 a = k \cot ka + \delta. \quad (8.49)$$

Unlike for the bound states, there is a smooth eigenfunction for any energy value as

$$\psi(x) = \begin{cases} 0, & \text{if } -\infty < x < 0; \\ C \sin k_0 x, & \text{if } 0 < x < a; \\ D \sin(kx + \delta), & \text{if } a < x < \infty. \end{cases} \quad (8.50)$$

By defining

$$A_0 = -\frac{C}{2i} \quad \text{and} \quad A = -\frac{De^{-2i\delta}}{2i} \quad (8.51)$$

we can write the solutions in the form

$$\psi(x) = \begin{cases} \text{wave traveling back and forth inside the well} \\ A_0 e^{-ik_0 x} - \overbrace{A_0 e^{+ik_0 x}}, & \text{if } 0 < x < a; \\ \underbrace{A e^{-ikx}}_{\text{incoming wave}} - \underbrace{A e^{2i\delta}}_{\text{outgoing wave with phase difference } 2\delta} e^{+ikx}, & \text{if } a < x < \infty. \end{cases} \quad (8.52)$$

See Fig. 8.5 with an example of a typical eigenfunction corresponding to an unbound state, with a phase shift and amplitude change due to the external potential.

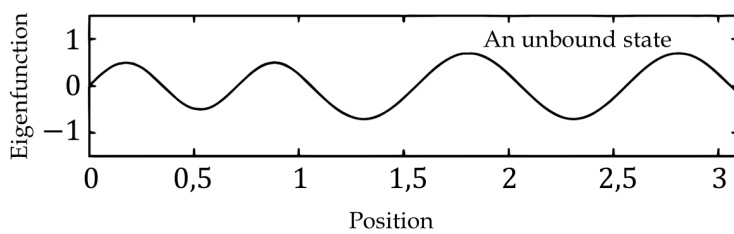


Figure 8.5: Example eigenfunction of the unbound state. The position is in units of a .

This lecture deepens the physical phenomena associated with quantum particle motion in external potentials. A quantum particle feels the influence of an external potential in a fundamentally different way from that of a classical particle. In particular, it can scatter back from a finite potential barrier such that only part of the wave propagates across it. The second important quantum property is that of tunneling – a quantum wave has a finite probability to penetrate through a finite barrier and reappear beyond it. This is classically forbidden, but theoretically possible although the probability becomes infinitesimally small for macroscopic objects and high barriers (as compared to the particle's energy).

9.1 Intended learning outcomes

- ▶ Understand the basic ideas of quantum scattering and tunneling
- ▶ Understand Bloch's theorem

9.2 Finite Potential Step - Scattering and Tunneling

The first nontrivial case is that of a finite potential barrier, see Fig. 9.1, where the QM particle can penetrate in and scatter from:

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

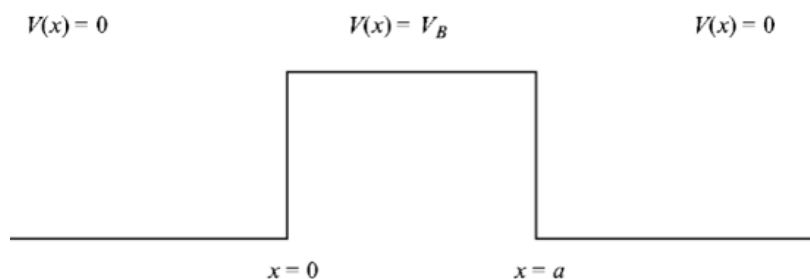


Figure 9.1: Finite potential barrier.

To obtain the full time-dependent solution of this problem, we would need to write the wave function in the form of Eq. (8.28). However, for now we consider the static (energy-based) solutions of the SE as in Lecture 8 and focus on the properties of the waves traveling in this potential.

First, to the left of the barrier

$$\psi_E''(x) = -k^2\psi_E(x); \quad E = \frac{\hbar^2 k^2}{2m}, \quad (9.2)$$

and the wave solution is

$$\psi_E(x) = A_I e^{ikx} + A_R e^{-ikx}, \quad (9.3)$$

where the intensity of the *incident* wave is $|A_I|^2$ and that of the *reflected* wave $|A_R|^2$. The incident and reflected directions are determined by the sign of k . Note that here in the 1D case you don't see the signs, but in general the argument is $\vec{k} \cdot \vec{r}$ which is positive for forward and negative for backward propagation.

When the energy of the incoming particle is larger than that of the barrier (classical crossing), we have

$$\psi_E''(x) = -k_B^2\psi_E(x); \quad E = \frac{\hbar^2 k_B^2}{2m} + V_B, \quad (9.4)$$

whose general solution is

$$\psi_E(x) = A e^{ik_B x} + A' e^{-ik_B x}. \quad (9.5)$$

For $E < V_B$, the region is classically forbidden (reflection), but the SE gives

$$\psi_E''(x) = \beta^2\psi_E(x); \quad E = \frac{\hbar^2 \beta^2}{2m} + V_B, \quad (9.6)$$

and the general solution becomes a decaying exponential

$$\psi_E(x) = B e^{-\beta x} + B' e^{\beta x}. \quad (9.7)$$

Finally, on the r.h.s. of the barrier (equals l.h.s.)

$$\psi_E(x) = A_T e^{ikx}; \quad k = \frac{\sqrt{2Em}}{\hbar}. \quad (9.8)$$

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

$$R = \frac{|A_R|^2}{|A_I|^2} \quad \text{and} \quad T = \frac{|A_T|^2}{|A_I|^2}. \quad (9.9)$$

These are called reflection and transmission probabilities, for which we have

$$R + T = 1. \quad (9.10)$$

We focus here on a particle whose energy is below the barrier:

$$\psi_E(x) = \begin{cases} A_I e^{+ikx} + A_R e^{-ikx}, & \text{if } -\infty < x < 0; \\ B e^{-\beta x} + B' e^{+\beta x}, & \text{if } 0 < x < a; \\ A_T e^{+ikx}, & \text{if } a < x < +\infty. \end{cases} \quad (9.11)$$

Continuity at $x = 0$ and a gives

$$\begin{aligned} A_I + A_R &= B + B' & \text{and} & \quad ikA_I - ikA_R = -\beta B + \beta B'; & (9.12) \\ B e^{-\beta a} + B' e^{+\beta a} &= A_T e^{ika} & \text{and} & \quad -\beta B e^{-\beta a} + \beta B' e^{+\beta a} = ikA_T e^{ika}, & (9.13) \end{aligned}$$

from which we can get the amplitudes as a function of B

$$2ikA_I = -(\beta - ik)B + (\beta + ik)B'; \quad (9.14)$$

$$A_T e^{ika} = \frac{2\beta}{\beta - ik} B e^{-\beta a} \quad \text{and} \quad B' = B e^{-2\beta a} \frac{\beta + ik}{\beta - ik}. \quad (9.15)$$

In the limit of a wide barrier where $e^{-2\beta a} \ll 1$ we can approximate that $B' \ll B$, i.e., $2ikA_I \approx -(\beta - ik)B$, which gives

$$A_T e^{ika} \approx -\frac{4ik\beta e^{-\beta a}}{(\beta - ik)^2} A_I, \quad (9.16)$$

and

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

Using the definitions

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

this can be written as

$$T \approx \frac{16E(V_B - E)}{V_B^2} e^{-2\beta a}. \quad (9.19)$$

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:

$$V(x) = -\alpha\delta(x), \quad (9.20)$$

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

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

(as previously discussed in Section 3.4), and the scale factor $\alpha > 0$ is the “strength” or “depth” of the potential well:

$$\int_{-\infty}^{\infty} V(x) dx = -\alpha. \quad (9.22)$$

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

With this potential function, the energy-eigenvalue SE in the position basis reads

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

The delta-function potential well supports both *bound* ($E < 0$) and *scattering* ($E > 0$) states. First, consider bound states with $x < 0$, where the SE is

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

This has the decaying solution

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

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

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

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

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

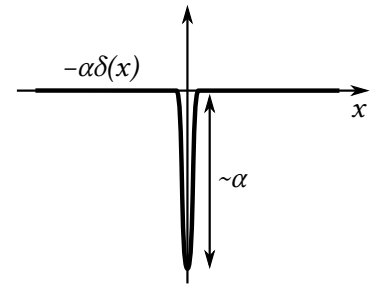


Figure 9.2: An approximation of the delta-function potential well with depth α .

1. ψ is always continuous
2. $\frac{d\psi}{dx}$ is continuous except at points where the potential is infinite

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

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

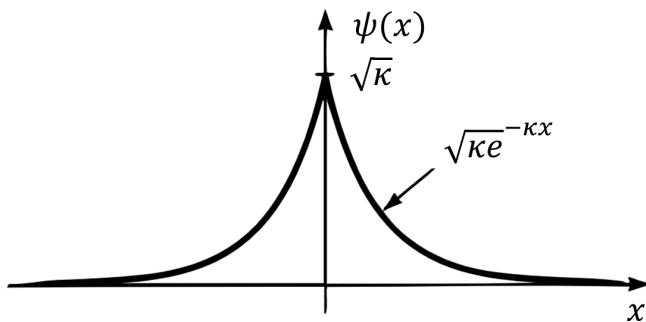


Figure 9.3: Bound state wave function for $E < 0$

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

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

L.h.s. term gives the jump in the derivative as

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

and due to the delta function

$$\Delta \left(\frac{d\psi}{dx} \right) = -\frac{2m\alpha}{\hbar^2} \psi(0). \quad (9.30)$$

Here

$$\frac{d\psi}{dx} = \begin{cases} -B\kappa e^{-\kappa x}, & \text{for } x > 0, \text{ so } \left. \frac{d\psi}{dx} \right|_+ = -B\kappa; \\ +B\kappa e^{+\kappa x}, & \text{for } x < 0, \text{ so } \left. \frac{d\psi}{dx} \right|_- = +B\kappa, \end{cases} \quad (9.31)$$

and thus

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

Normalization gives

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2|B|^2 \int_0^{\infty} e^{-2\kappa x} dx = \frac{|B|^2}{\kappa} = 1. \quad (9.33)$$

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

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

For the scattering states $E > 0$

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

and the general solution for $x < 0$ is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \quad (9.36)$$

and for $x > 0$

$$\psi(x) = Fe^{ikx} + Ge^{-ikx}. \quad (9.37)$$

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

$$\frac{d\psi}{dx} = \begin{cases} ik(Fe^{ikx} - Ge^{-ikx}), & \text{for } x > 0, \text{ so } \left. \frac{d\psi}{dx} \right|_+ = ik(F - G); \\ ik(Ae^{ikx} - Be^{-ikx}), & \text{for } x < 0, \text{ so } \left. \frac{d\psi}{dx} \right|_- = ik(A - B), \end{cases} \quad (9.38)$$

which gives the jump

$$\Delta\psi' \Big|_{x=0} = ik(F - G - A + B) = -\frac{2m\alpha}{\hbar^2}\psi(0). \quad (9.39)$$

Because the plane waves are *not normalizable in free space*, these equations don't have unique solutions. We have to assume a wave coming from a given direction, e.g. from left to right, see Fig. 9.4.

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

$$B = \frac{i\beta}{1 - i\beta}A \quad F = \frac{1}{1 - i\beta}A \quad (9.40)$$

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

These can now be used to refine the corresponding reflection and transmission coefficients $R + T = 1$

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

9.4 Scattering Matrix

The results based on specific potentials can be generalized to incoming and outgoing waves for any potential shape which can

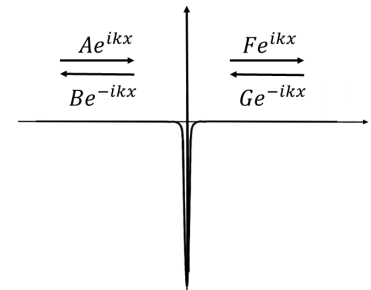


Figure 9.4: Directions for the given waves.

be divided into zero and non-zero regions (see Fig. 9.5).

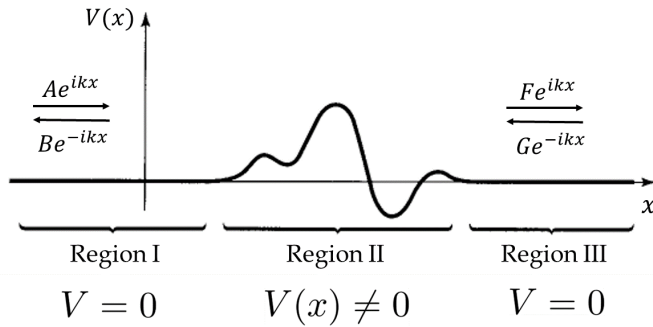


Figure 9.5: An example potential with zero and non-zero regions.

For the scattering sites $E > 0$

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

and the general solutions for $V = 0$ are as before shown in Eqs. (9.36) and (9.37). The general solution in between (Region II in Fig. 9.5) has to be of the form (why?)

$$\psi(x) = Cf(x) + Dg(x), \quad (9.44)$$

where $f(x)$ and $g(x)$ are any two linearly independent *particular* solutions of the (static) SE for the given $V(x)$.

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

$$B = S_{11}A + S_{12}G; \quad (9.45)$$

$$F = S_{21}A + S_{22}G, \quad (9.46)$$

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

$$S = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}, \quad (9.47)$$

which is the scattering (S) matrix, for which

$$\begin{bmatrix} B \\ F \end{bmatrix} = S \begin{bmatrix} A \\ G \end{bmatrix}. \quad (9.48)$$

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

$$R_l = \frac{|B|^2}{|A|^2} \Big|_{G=0} = |S_{11}|^2; \quad T_l = \frac{|F|^2}{|A|^2} \Big|_{G=0} = |S_{21}|^2, \quad (9.49)$$

and from the right, $A = 0$:

$$R_r = \frac{|F|^2}{|G|^2} \Big|_{A=0} = |S_{22}|^2; \quad T_r = \frac{|B|^2}{|G|^2} \Big|_{A=0} = |S_{22}|^2. \quad (9.50)$$

The existence of possible bound states is in diverging components of the S-matrix (maybe homework).

9.5 Bloch's theorem

An important special case is that of a periodic potential $V(x + a) = V(x)$, see Fig. 9.6.

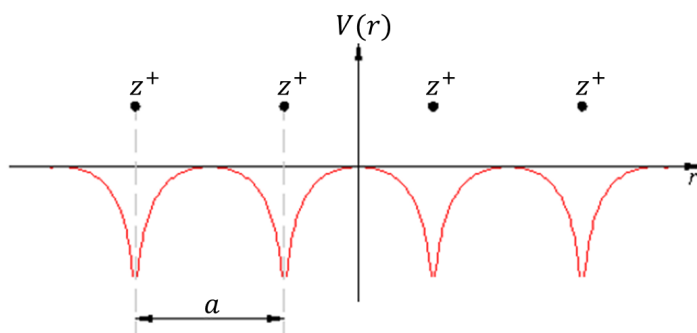


Figure 9.6: Example of a periodic potential.

Theorem 9.5.1 (Bloch's theorem) *Any wave function that is a 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 $n = 0, \pm 1, \dots, \pm \frac{N}{2}$ 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.

This lecture deals with the fundamental statistical properties of quantum particles. In the traditional classification there are two types of particles, namely bosons and fermions. They differ by how their corresponding quantum states can be occupied, or more precisely what the symmetries of the corresponding wave functions are corresponding to many such particles. Another way of separating between bosons and fermions is by their spin, which is embodied in the spin-statistics theorem below. In 2D there also exist third type of quantum particles called anyons, but they will not be discussed here.

10.1 Intended learning outcomes

- ▶ Understand the difference between bosons and fermions
- ▶ Understand how in general to construct many-particle boson and fermion states
- ▶ Understand creation and annihilation operators for bosons and fermions

10.2 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

$$|\Psi(x_1, x_2, t)|^2 dx_1 dx_2. \quad (10.1)$$

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

$$|\Psi(x_1, x_2, t)|^2 = |\Psi(x_2, x_1, t)|^2, \quad (10.2)$$

which means that

$$\Psi(x_1, x_2, t) = \Psi(x_2, x_1, t)e^{i\delta}, \quad (10.3)$$

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

$$\Psi^S(x) \propto \psi_n(x_1)\psi'_{n'}(x_2) + \psi_n(x_2)\psi'_{n'}(x_1); \quad (10.4)$$

$$\Psi^A(x) \propto \psi_n(x_1)\psi'_{n'}(x_2) - \psi_n(x_2)\psi'_{n'}(x_1). \quad (10.5)$$

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

$$E = E_n + E_{n'} = (n + n' + 1)\hbar\omega. \quad (10.6)$$

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

$$\Psi_1^{(D)}(x_p, x_q, t) = \psi_n(x_p)\psi'_{n'}(x_q)e^{-i(E_n+E_{n'})t/\hbar}; \quad (10.7)$$

$$\Psi_2^{(D)}(x_p, x_q, t) = \psi_n(x_q)\psi'_{n'}(x_p)e^{-i(E_n+E_{n'})t/\hbar}, \quad (10.8)$$

or a linear combination as

$$\Psi^{(D)}(x_p, x_q, t) = c_1\Psi_1^{(D)}(x_p, x_q, t) + c_2\Psi_2^{(D)}(x_p, x_q, t). \quad (10.9)$$

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

$$\Psi^{(S)}(x_p, x_q, t) = \frac{1}{\sqrt{2}} [\psi_n(x_p)\psi'_{n'}(x_q) + \psi_n(x_q)\psi'_{n'}(x_p)] e^{-i(E_n+E_{n'})t/\hbar}; \quad (10.10)$$

$$\Psi^{(A)}(x_p, x_q, t) = \frac{1}{\sqrt{2}} [\psi_n(x_p)\psi'_{n'}(x_q) - \psi_n(x_q)\psi'_{n'}(x_p)] e^{-i(E_n+E_{n'})t/\hbar}. \quad (10.11)$$

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

$$\Psi_{1,2}^{(D)}(x_0, x_0, t) = \psi_n(x_0)\psi'_{n'}(x_0)e^{-i(E_n+E_{n'})t/\hbar} \quad (10.12)$$

For two identical particles the symmetrical unentangled WF is

$$\Psi_{1,2}^{(S)}(x_0, x_0, t) = \sqrt{2}\psi_n(x_0)\psi'_{n'}(x_0)e^{-i(E_n+E_{n'})t/\hbar} \quad (10.13)$$

and the antisymmetrical one

$$\Psi^{(A)}(x_0, x_0, t) = 0 \quad (10.14)$$

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

$$x = x_p - x_q \quad \text{and} \quad X = \frac{x_p + x_q}{2}. \quad (10.15)$$

The corresponding WFs can be easily constructed (homework) and the probability density functions (PDF) are plotted in Fig. 10.1 for the symmetrical (S) and antisymmetrical (A) WFs of two identical particles and (unentangled) distinguishable particles (D)

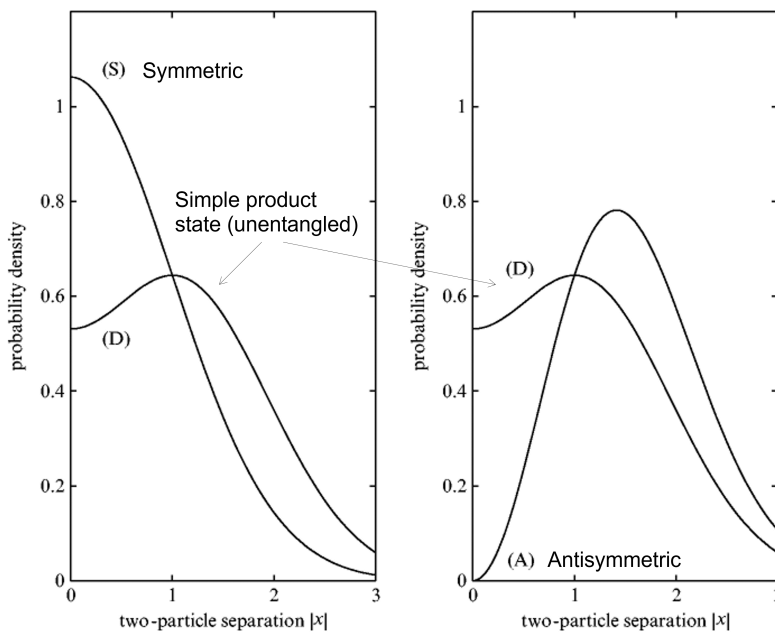


Figure 10.1: Probability density functions for the 1D QHO in the symmetrical (S), antisymmetrical (A), and unentangled (D) cases.

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 10.2.1 (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.

10.3 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 P_{ij} by

$$P_{ij}|k_1, k_2, \dots, k_i, k_j, \dots, k_N\rangle = |k_1, k_2, \dots, k_j, k_i, \dots, k_N\rangle. \quad (10.16)$$

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

$$\sum_P P|k_1, k_2, \dots, k_N\rangle := \sum \text{all } N! \text{ permutations of momenta in } |k_1, k_2, \dots, k_N\rangle. \quad (10.17)$$

For example,

$$\begin{aligned} \sum_P P|k_1, k_2, k_3\rangle = \{ & |k_1, k_2, k_3\rangle + |k_2, k_1, k_3\rangle + |k_1, k_3, k_2\rangle \\ & + |k_3, k_2, k_1\rangle + |k_3, k_1, k_2\rangle + |k_2, k_3, k_1\rangle\}. \end{aligned} \quad (10.18)$$

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:

$$n_i = \text{number of particles with momentum } k_i; \quad (10.19)$$

$$N = \sum_{i=1}^N n_i = \text{total number of particles}. \quad (10.20)$$

Thus there are exactly $\frac{N!}{\prod_{\alpha=1}^N n_{\alpha}!}$ different kets in $\sum_P P|k_1, k_2, \dots, k_N\rangle$.

Using orthonormality of the basis functions

$$\langle k_a, k_b, \dots, k_l | k'_a, k'_b, \dots, k'_l \rangle = \delta_{k_a, k'_a} \delta_{k_b, k'_b} \times \dots \times \delta_{k_l, k'_l} \quad (10.21)$$

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

$$|k_1, k_2, \dots, k_N\rangle^{(S)} = \left(\frac{N!}{\prod_{\alpha=1}^N n_{\alpha}!} \right) \sum_P P|k_1, k_2, \dots, k_N\rangle, \quad (10.22)$$

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

$$\hat{1}^{(S)} = \frac{1}{N!} \sum_{k_1, k_2, \dots, k_N} \left(\prod_{\alpha=1}^N n_{\alpha}! \right) |k_1, k_2, \dots, k_N\rangle^{(S)} \langle k_1, k_2, \dots, k_N|^{(S)}. \quad (10.23)$$

10.4 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 P_{ij} as in Eq. (10.16). Likewise, sum over all the permutations includes all possible combinations of the wave vectors as in Eq. (10.17).

The antisymmetric momentum eigenstates can be written as

$$|k_1, k_2, \dots, k_N\rangle^{(A)} = \frac{1}{\sqrt{N!}} \sum_P (-1)^P P |k_1, \dots, k_N\rangle, \quad (10.24)$$

where P is the number of permutations (changes)

For example,

$$\begin{aligned} \sum_P (-1)^P P |k_1, k_2, k_3\rangle &= \{|k_1, k_2, k_3\rangle - |k_2, k_1, k_3\rangle - |k_1, k_3, k_2\rangle \\ &\quad - |k_3, k_2, k_1\rangle + |k_3, k_1, k_2\rangle + |k_2, k_3, k_1\rangle\}. \end{aligned} \quad (10.25)$$

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 $\langle r_1, r_2, \dots, r_N | k_1, k_2, \dots, k_N \rangle^{(A)}$ can be written as the *Slater determinant*

$$\langle r_1, r_2, \dots, r_N | k_1, k_2, \dots, k_N \rangle^{(A)} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \langle r_1 | k_1 \rangle & \langle r_1 | k_2 \rangle & \cdots & \langle r_1 | k_N \rangle \\ \langle r_2 | k_1 \rangle & \langle r_2 | k_2 \rangle & \cdots & \langle r_2 | k_N \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle r_N | k_1 \rangle & \langle r_N | k_2 \rangle & \cdots & \langle r_N | k_N \rangle \end{vmatrix}, \quad (10.26)$$

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.

10.5 Annihilation and Creation Operators

Consider first the case of **fermions** (antisymmetric WFs). The creation operator C_α^\dagger is defined by the relations

$$C_\alpha^\dagger|0\rangle = |\alpha\rangle := |\phi_\alpha\rangle; \quad (10.27)$$

$$C_\alpha^\dagger|\beta\rangle = C_\alpha^\dagger C_\beta^\dagger|0\rangle = |\alpha\beta\rangle = -|\beta\alpha\rangle; \quad (10.28)$$

$$C_\alpha^\dagger|\beta\gamma\rangle = C_\alpha^\dagger C_\beta^\dagger C_\gamma^\dagger|0\rangle = |\alpha\beta\gamma\rangle, \quad (10.29)$$

etc.

The Pauli exclusion principle requires that

$$C_\alpha^\dagger|\alpha \cdots\rangle = 0. \quad (10.30)$$

The adjoint operator $C_\alpha := \left(C_\alpha^\dagger\right)^\dagger$ defines the annihilation operator

$$C_\alpha|\alpha\rangle = |0\rangle; \quad (10.31)$$

$$C_\alpha|0\rangle = 0. \quad (10.32)$$

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

$$\{C_\alpha, C_\beta^\dagger\} := C_\alpha C_\beta^\dagger + C_\beta^\dagger C_\alpha = \delta_{\alpha\beta} \mathbf{I}, \quad (10.33)$$

and the number operator is given by

$$N = \sum_\alpha C_\alpha^\dagger C_\alpha. \quad (10.34)$$

Similarly, for the case of **bosons** (symmetric WFs) the creation operator a_α^\dagger is defined by the relations

$$a_\alpha^\dagger|0\rangle = |\phi_\alpha\rangle = |0, 0, \dots, n_\alpha = 1, 0, \dots\rangle; \quad (10.35)$$

$$a_\alpha^\dagger|n_1, n_2, \dots, n_\alpha, \dots\rangle \propto |n_1, n_2, \dots, n_\alpha + 1, \dots\rangle, \quad (10.36)$$

and the annihilation operator $a_\alpha := \left(a_\alpha^\dagger\right)^\dagger$

$$a_\alpha|\phi_\alpha\rangle = |0\rangle; \quad (10.37)$$

$$a_\alpha|n_1, n_2, \dots, n_\alpha, \dots\rangle \propto |n_1, n_2, \dots, n_\alpha - 1, \dots\rangle \quad (n_\alpha > 0); \quad (10.38)$$

$$a_\alpha|n_1, n_2, \dots, n_\alpha = 0, \dots\rangle = 0. \quad (10.39)$$

The number operator is given by

$$N = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}, \quad (10.40)$$

and

$$a_{\alpha} |n_1, n_2, \dots, n_{\alpha}, \dots\rangle = (n_{\alpha})^{\frac{1}{2}} |n_1, n_2, \dots, n_{\alpha} - 1, \dots\rangle; \quad (10.41)$$

$$a_{\alpha}^{\dagger} |n_1, n_2, \dots, n_{\alpha}, \dots\rangle = (n_{\alpha} + 1)^{\frac{1}{2}} |n_1, n_2, \dots, n_{\alpha} + 1, \dots\rangle. \quad (10.42)$$

$$(10.43)$$

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

$$\left[a_{\alpha}, a_{\beta}^{\dagger} \right] := a_{\alpha} a_{\beta}^{\dagger} - a_{\beta}^{\dagger} a_{\alpha} = \delta_{\alpha\beta} \mathbf{I}. \quad (10.44)$$

In quantum (and even classical) 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 considering a simple (solvable) case which has been only slightly perturbed, it is possible to develop a systematic expansion in terms of the eigenfunctions of that solvable system. This is the basis of perturbation theory, whose time-independent version is presented here.

11.1 Intended learning outcomes

- ▶ Learn how to form an orthonormal basis for any complete set of eigenfunctions
- ▶ Understand the idea behind perturbation theory

The first step in developing perturbation theory is to make sure that there is a complete, orthonormal set of eigenfunctions available. To this end, the Gram–Schmidt orthogonalization method may be needed.

11.2 Perturbation Theory

Gram–Schmidt Orthogonalization

Assume that we have a complete set of *linearly independent* eigenvectors that span a vector space (or Hilbert space), but they are not orthonormal.

Assume for simplicity that the set is given by

$$S = \{|v_1\rangle, |v_2\rangle, \dots, |v_n\rangle\}, \quad (11.1)$$

and we want to create a new orthogonal set

$$S_{\perp} = \{|u_1\rangle, |u_2\rangle, \dots, |u_n\rangle\}, \quad (11.2)$$

that spans the same space as S . This is called the Gram-Schmidt process.

Define a projection operator

$$\hat{P}_u(v) := \frac{\langle u|v\rangle}{\langle u|u\rangle}|u\rangle. \quad (11.3)$$

The GS process simply comprises repeated orthogonal projections, subtracting the non-orthogonal parts and finally normalizing, see Fig. 11.1 as well:

$$|u_1\rangle = |v_1\rangle, \quad |e_1\rangle = \frac{|u_1\rangle}{\|u_1\|}; \quad (11.4)$$

$$|u_2\rangle = |v_2\rangle - \hat{P}_{u_1}(v_2), \quad |e_2\rangle = \frac{|u_2\rangle}{\|u_2\|}; \quad (11.5)$$

$$|u_3\rangle = |v_3\rangle - \hat{P}_{u_1}(v_3) - \hat{P}_{u_2}(v_3), \quad |e_3\rangle = \frac{|u_3\rangle}{\|u_3\|}; \quad (11.6)$$

$$|u_4\rangle = |v_4\rangle - \hat{P}_{u_1}(v_4) - \hat{P}_{u_2}(v_4) - \hat{P}_{u_3}(v_4), \quad |e_4\rangle = \frac{|u_4\rangle}{\|u_4\|}. \quad (11.7)$$

The final orthonormal basis set is simply thus

$$S_{\perp}^N = \{|e_1\rangle, |e_2\rangle, \dots, |e_n\rangle\}. \quad (11.8)$$

Time-Independent Perturbation Theory

Assume that we have solved the SE for a given external potential such that

$$\hat{H}^0 \psi_n^0 = E_n^0 \psi_n^0, \quad (11.9)$$

and the energy eigenfunctions form an orthonormal set

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm}, \quad (11.10)$$

which can be generated by the Gram–Schmidt process if need be.

If the new problem is exactly solvable, we have

$$\hat{H} \psi_n = E_n \psi_n. \quad (11.11)$$

If however the perturbation is “small” (see Fig. 11.2), we could try writing

$$\hat{H} = \hat{H}^0 + \lambda \hat{H}', \quad (11.12)$$

where now $\lambda \ll 1$, such that we can (formally) expand

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots \quad (11.13)$$

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots, \quad (11.14)$$

where the superscripts denote the n th order corrections to the unperturbed state denoted by 0. This expression is inserted into

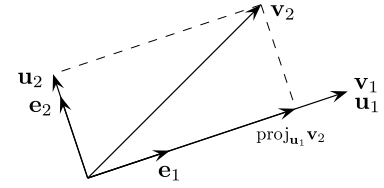


Figure 11.1: The first two steps of the Gram–Schmidt process [1].

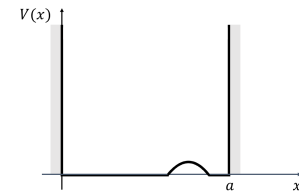


Figure 11.2: Small perturbation on $V(x)$.

the modified SE to get

$$H^0 \psi_n^0 + \lambda (H^0 \psi_n^1 + H' \psi_n^0) + \lambda^2 (H^0 \psi_n^2 + H' \psi_n^1) + \dots \quad (11.15)$$

$$= E_n^0 \psi_n^0 + \lambda (E_n^0 \psi_n^1 + E_n^1 \psi_n^0) + \lambda^2 (E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0) + \dots \quad (11.16)$$

To lowest order this gives just the unmodified SE. To first order

$$H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0, \quad (11.17)$$

and to second order

$$H^0 \psi_n^2 + H' \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0. \quad (11.18)$$

Taking the inner product of the first equation with ψ_n^0 gives the first-order correction as

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle. \quad (11.19)$$

Rewriting the lowest order correction as

$$(H^0 - E_n^0) \psi_n^1 = - (H' - E_n^1) \psi_n^0, \quad (11.20)$$

and expanding the first-order correction in the original SE basis gives

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 = - (H' - E_n^1) \psi_n^0. \quad (11.21)$$

Taking the inner product with ψ_l^0

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \langle \psi_l^0 | \psi_m^0 \rangle = - \langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \langle \psi_l^0 | \psi_n^0 \rangle, \quad (11.22)$$

and orthogonality gives

$$c_m^{(n)} = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}, \quad (11.23)$$

which gives the first-order correction to the original SE basis as

$$\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0. \quad (11.24)$$

To get the second-order corrections, we use the second-order

equation and operate with

$$\langle \psi_n^0 | H^0 \psi_n^2 \rangle + \langle \psi_n^0 | H' \psi_n^1 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle, \quad (11.25)$$

where

$$\langle \psi_n^0 | \psi_n^1 \rangle = \sum_{m \neq n} c_m^{(n)} \langle \psi_n^0 | \psi_m^0 \rangle = 0, \quad (11.26)$$

and thus

$$E_n^2 = \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}. \quad (11.27)$$

In degenerate case, a general expansion in terms of eigenvectors of the original SE should be used.

While the full time-dependent SE gives a complete solution to the 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 called *pictures* and they are the main topic in this Lecture. First, the adiabatic theorem will be briefly explained and at the end the density matrix will be introduced.

12.1 Intended learning outcomes

- ▶ Understand the basis of the adiabatic theorem
- ▶ Understand the different dynamical pictures
- ▶ Become familiar with the important concept of a density matrix (operator)

12.2 Time Dependence

Adiabatic Theorem

Assume that we have a system that “very slowly” evolves in time s.t. the Hamiltonian $\hat{H}^i \rightarrow \hat{H}^f$ as in Fig. 12.1.

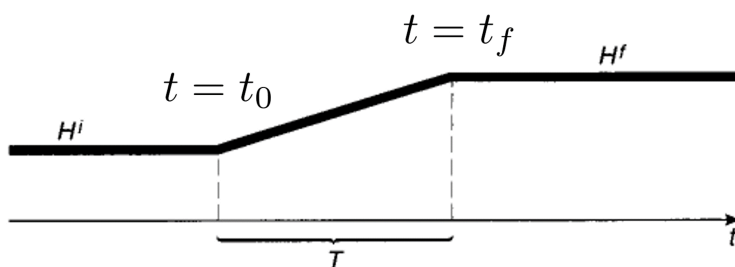


Figure 12.1: Adiabatic process evolution.

Adiabatic processes carry the system from an initial eigenstate of $\hat{H}^i(t = t_0)$ to that of the final Hamiltonian $\hat{H}^f(t = t_f)$.

For example, if for the infinite well the wall distance is adiabatically increased from a to $2a$ (see Fig. 12.2):

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

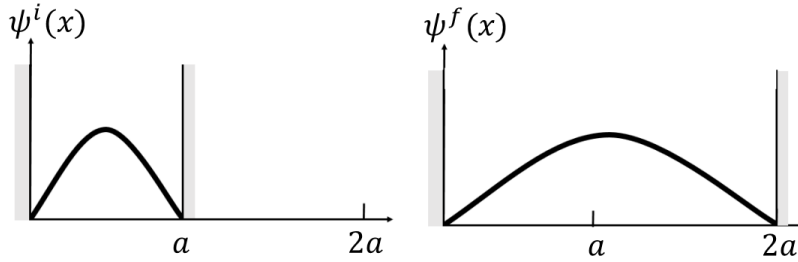


Figure 12.2: Increasing the infinite well wall distance adiabatically.

For rapid (non-adiabatic) processes the final state is some combination of final eigenstates.

While usually in quantum mechanics an overall phase prefactor $e^{i\theta}$ is not measurable, a time-dependent Hamiltonian may make it possible to measure. Such a prefactor is called the *Berry phase* and it is discussed in Appendix A.1.

12.3 Temporal Dependence of Operators

The *formulation of quantum dynamics is not unique for the states and operators*. Consider the expectation value of some (Hermitian) operator

$$\langle \hat{A}(t) \rangle = \langle \psi(t) | \hat{A} | \psi(t) \rangle = \langle \hat{U}(t) \psi(0) | \hat{A} | \hat{U}(t) \psi(0) \rangle \quad (12.1)$$

$$= \langle \psi(0) | \hat{U}^\dagger(t) \hat{A} \hat{U}(t) | \psi(0) \rangle \quad (12.2)$$

$$= \left(\psi(0) | \hat{U}^\dagger(t) \right) \hat{A} \left(\hat{U}(t) | \psi(0) \right) \quad (12.3)$$

$$= \langle \psi(0) | \left(\hat{U}^\dagger(t) \hat{A} \hat{U}(t) \right) | \psi(0) \rangle, \quad (12.4)$$

where the time-evolution operator from the Schrödinger equation propagates the wave function

$$\Psi_n(x, t) = \hat{U}(t) \psi_n(x, t), \quad (12.5)$$

and follows the equation of motion

$$i\hbar \frac{\partial \hat{U}(t, t_0)}{\partial t} = \hat{H}(t) \hat{U}(t, t_0) \quad (12.6)$$

giving

$$\hat{U}(t, t_0) = e^{-\frac{i}{\hbar} \int_{t_0}^t dt' \hat{H}(t')}. \quad (12.7)$$

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

$$\langle \hat{A}(t) \rangle = \left(\langle \psi(0) | \hat{U}^\dagger(t) \right) \hat{A} \left(\hat{U}(t) | \psi(0) \right), \quad (12.8)$$

and where the operator(s) evolve in time but states stay the same is the *Heisenberg picture*:

$$\langle \hat{A}(t) \rangle = \langle \psi(0) | \left(\hat{U}^\dagger(t) \hat{A} \hat{U}(t) \right) | \psi(0) \rangle. \quad (12.9)$$

Schrödinger Picture

The time evolution of the state is governed by

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle_S = \hat{H} |\psi(t)\rangle_S, \quad (12.10)$$

or equivalently

$$|\psi(t)\rangle_S = \hat{U}(t, t_0) |\psi(t_0)\rangle_S. \quad (12.11)$$

For operators (expectation values)

$$i\hbar \frac{\partial}{\partial t} \langle \psi(t) | \hat{A} | \psi(t) \rangle_S = i\hbar \left(\langle \dot{\psi}(t) | \hat{A} | \psi(t) \rangle_S + \langle \psi(t) | \dot{\hat{A}} | \psi(t) \rangle_S \right) \quad (12.12)$$

$$= \langle \psi(t) | \hat{A} \hat{H} | \psi(t) \rangle_S - \langle \psi(t) | \hat{H} \hat{A} | \psi(t) \rangle_S \quad (12.13)$$

$$= \langle [\hat{A}, \hat{H}] \rangle_S. \quad (12.14)$$

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

Heisenberg Picture

In the Heisenberg picture (HP), the states do not evolve in time but the operators (expectation values) do, and we can write

$$\hat{A}_H(t) = \hat{U}^\dagger(t, t_0) \hat{A}_S \hat{U}(t, t_0), \quad (12.15)$$

which agree at time t_0 . The wave functions are related by

$$|\psi(t)\rangle_S = \hat{U}(t, t_0) |\psi\rangle_H. \quad (12.16)$$

The operators depend on time now and their equation of motion is given by

$$\frac{\partial \hat{A}_H}{\partial t} = \frac{\partial \hat{U}^\dagger \hat{A}_S \hat{U}}{\partial t} \quad (12.17)$$

$$= \frac{i}{\hbar} \left(\hat{U}^\dagger \hat{H} \hat{A}_S \hat{U} - \hat{U}^\dagger \hat{A}_S \hat{H} \hat{U} \right) \quad (12.18)$$

$$= \frac{i}{\hbar} (\hat{H}_H \hat{A}_H - \hat{A}_H \hat{H}_H) \quad (12.19)$$

$$= -\frac{i}{\hbar} [\hat{A}, \hat{H}]_H. \quad (12.20)$$

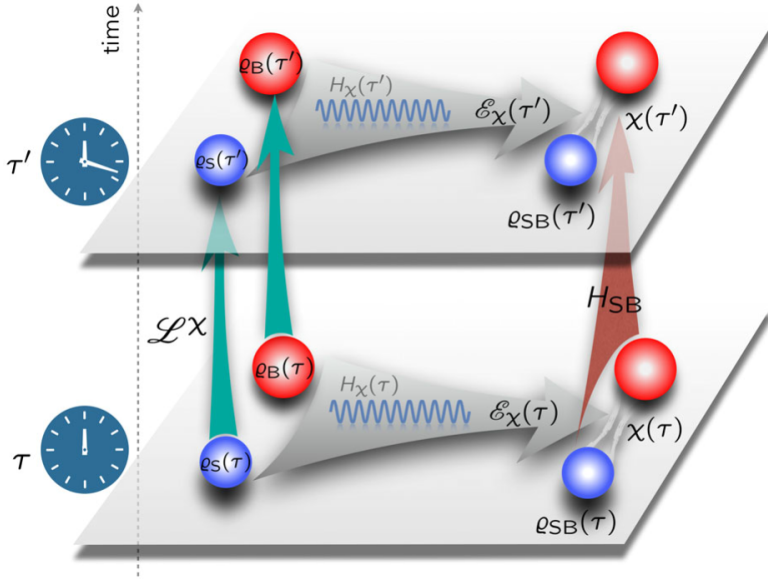


Figure 12.3: Description of the correlation picture. At any time τ (or τ_0), a correlating transformation \mathcal{E}_χ transforms an uncorrelated state $\rho_S \otimes \rho_B$ to a correlated state $\rho_{SB} = \rho_S \otimes \rho_B + \chi$, at the same instant of time, due to an abstract correlation-dependent 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}^χ constructed from H_{SB} , the generator of the total system dynamics in the Schrödinger picture.

Note that for time-independent Hamiltonian

$$\hat{H}_H = \hat{U}^\dagger \hat{H} \hat{U} = \hat{H}. \quad (12.21)$$

There is also an *interaction (Dirac) picture*, which is used when the system Hamiltonian can be divided into two parts as (in Schrödinger picture)

$$\hat{H}_S = \hat{H}_S^0 + \hat{H}_S^I, \quad (12.22)$$

where the first part is “easy” (usually solvable). Then a state vector in the interaction picture is given by

$$|\psi(t)\rangle_I = e^{i\hat{H}_S^0 t/\hbar} |\psi(t)\rangle_S. \quad (12.23)$$

An operator in the interaction picture is defined by

$$\hat{A}_I(t) = e^{i\hat{H}_S^0 t/\hbar} \hat{A}_S e^{-i\hat{H}_S^0 t/\hbar}. \quad (12.24)$$

Recently a correlation picture (transformation) has been introduced for open quantum systems [2], see Fig. 12.3.

12.4 Density Matrix

The formulation of QM for systems of many degrees of freedom can also be done using the density matrix, which is a representation of the density operator (in what picture?)

$$\hat{\rho}(t) = |\psi(t)\rangle\langle\psi(t)|. \quad (12.25)$$

Consider a general wave function expanded in orthonormal basis (e.g. energy basis)

$$|\psi(t)\rangle = \sum_n c_n(t) |n\rangle. \quad (12.26)$$

The expectation value of an operator \hat{A} is

$$\langle \hat{A}(t) \rangle = \sum_{n,m} c_n(t) c_m^*(t) \langle m | \hat{A} | n \rangle, \quad (12.27)$$

and the elements of the density matrix can be obtained with the help of the decomposition

$$\hat{\rho}(t) = \sum_{n,m} c_n(t) c_m^*(t) |n\rangle \langle m|. \quad (12.28)$$

They are defined by

$$\rho_{n,m}(t) := c_n(t) c_m^*(t). \quad (12.29)$$

This gives the important result that

$$\langle \hat{A} \rangle = \sum_{n,m} c_n(t) c_m^*(t) \langle m | \hat{A} | n \rangle \quad (12.30)$$

$$= \sum_{n,m} \rho_{n,m} \langle m | \hat{A} | n \rangle \quad (12.31)$$

$$= \sum_{n,m} A_{m,n} \rho_{n,m}(t) \quad (12.32)$$

$$= \text{Tr} (\hat{A} \hat{\rho}(t)). \quad (12.33)$$

Trace operator

Tr is the trace operator. It is the sum of the diagonal terms of a given matrix.

Properties of the density matrix (operator):

- ▶ It is Hermitian (obviously)
- ▶ It is normalized, $\text{Tr} \hat{\rho}(t) = 1$
- ▶ It is bound from below and above by mixed and pure states: $\text{Tr} \hat{\rho}^2(t) = 1$ for pure states and $\text{Tr} \hat{\rho}^2(t) < 1$ for mixed states
- ▶ For mixed states, we can write in general (in a non-interacting many-particle system)

$$|\psi_i\rangle = \sum_n c_n^i |n\rangle. \quad (12.34)$$

- ▶ The density matrix elements are

$$\rho_{n,m} = \langle n | \hat{\rho} | m \rangle = \sum_i \langle n | \psi_i \rangle \langle \psi_i | m \rangle \quad (12.35)$$

$$= \sum_i \sum_{n,m} c_n^i (c_m^i)^*. \quad (12.36)$$

Here the density matrix elements represent the *eigenstate coefficients*

averaged over the mixture. Diagonal elements give the probability of occupying a quantum state $|n\rangle$, i.e., the populations. Off-diagonal elements are complex (in general) and have time-dependent phase factors that describe the *evolution of coherent superpositions of the eigenstates*.

Temporal Evolution of The Density Matrix

Using the SE it is easy to show that (homework)

$$\frac{\partial \hat{\rho}(t)}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}], \quad (12.37)$$

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

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t), \quad (12.38)$$

where the time evolution operator is defined in Eq. (12.7).

The average of an operator can be computed either in the Schrödinger picture (propagating the density matrix) or in the Heisenberg picture (propagating the operator):

$$\langle \hat{A}(t) \rangle = \text{Tr} (\hat{A}\hat{\rho}(t)) \quad (12.39)$$

$$= \text{Tr} (\hat{A}\hat{U}(t)\hat{\rho}(0)\hat{U}^\dagger(t)) \quad (12.40)$$

$$= \text{Tr} (\hat{U}^\dagger(t)\hat{A}\hat{U}(t)\hat{\rho}(0)) \quad (12.41)$$

$$= \text{Tr} (\hat{A}(t)\hat{\rho}(0)), \quad (12.42)$$

where in Eq. (12.41), we have used the cyclic property of the trace: $\text{Tr} (\hat{A}\hat{B}\hat{C}) = \text{Tr} (\hat{C}\hat{A}\hat{B}) = \text{Tr} (\hat{B}\hat{C}\hat{A})$.

For a time-independent Hamiltonian the dynamics of the density matrix becomes simple as

$$\rho_{n,m}(t) = \langle n|\hat{\rho}(t)|m\rangle = \langle n|\hat{U}(t)|\psi(0)\rangle\langle\psi(0)|\hat{U}^\dagger(t)|m\rangle, \quad (12.43)$$

and thus for energy eigenfunctions

$$\rho_{n,m}(t) = e^{-i(E_m - E_n)t/\hbar} \rho_{n,m}(0). \quad (12.44)$$

This means that the *populations are time-independent* but the *coherences oscillate* in time with a frequency corresponding to the level splitting.

Density Matrix in the Interaction Picture

In the interaction picture (IP) we wrote, see Eq. (12.22):

$$\hat{H}_S = \hat{H}_S^0 + \hat{H}_S^I, \quad (12.45)$$

and the evolution of the state vector is given by

$$|\psi(t)\rangle_I = e^{-i\hat{H}_S^0 t/\hbar} |\psi(t)\rangle_S =: \hat{U}_0^\dagger(t) |\psi(t)\rangle_S. \quad (12.46)$$

This means that the density matrix in the IP can be written as

$$\hat{\rho}_I(t) = \hat{U}_0^\dagger(t) \rho_S \hat{U}_0(t). \quad (12.47)$$

In analogy to the Schrödinger picture case, the equation of motion then becomes

$$\frac{\partial \hat{\rho}_I(t)}{\partial t} = -\frac{i}{\hbar} [\hat{H}_I(t), \hat{\rho}_I(t)], \quad (12.48)$$

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

References

- [1] Wikimedia Common, Gustavb. *File:Gram–Schmidt process.svg* — *Wikimedia Commons, the free media repository*. [Online; accessed 25th September 2022]. 2020. URL: https://commons.wikimedia.org/w/index.php?title=File:Gram%5C%E2%5C%80%5C%93Schmidt_process.svg&oldid=509222105 (cited on page 71).
- [2] S. Alipour et al. ‘Correlation-Picture Approach to Open-Quantum-System Dynamics’. In: *Phys. Rev. X* 10 (4 Nov. 2020), p. 041024. DOI: [10.1103/PhysRevX.10.041024](https://doi.org/10.1103/PhysRevX.10.041024) (cited on page 77).

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

A.1 Geometric and Berry Phases

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

$$\hat{H}\psi_n(x) = E_n\psi_n(x) \quad (\text{A.1})$$

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

$$\Psi_n(x, t) = \psi_n(x)e^{\frac{iE_nt}{\hbar}}. \quad (\text{A.2})$$

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

$$\hat{H}(t)\psi_n(x, t) = E_n(t)\psi_n(x, t). \quad (\text{A.3})$$

According to the adiabatic theorem (see Section 12.2), the system will remain at the n th eigenstate even with time dependence:

$$\psi_n(x, t) = \hat{U}(t)\psi_n(x, t_0) \quad (\text{A.4})$$

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

$$i\hbar \frac{\partial \hat{U}(t, t_0)}{\partial t} = \hat{H}(t)\hat{U}(t, t_0) \quad (\text{A.5})$$

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

$$\hat{U}(t, t_0) = e^{-i \int_{t_0}^t dt' \hat{H}(t')/\hbar} \quad (\text{A.6})$$

Operating on the eigenstates gives simply that

$$\Psi_n(x, t) = \psi_n(x, t_0) e^{-i \int_{t_0}^t dt' E_n(t')/\hbar} e^{i\gamma_n(t)} \quad (\text{A.7})$$

The term

$$\theta_n(x, t) = - \int_{t_0}^t dt' \frac{E_n(t')}{\hbar} \quad (\text{A.8})$$

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

$$i\hbar \left[\frac{\partial \psi_n}{\partial t} e^{i\theta_n} e^{i\gamma_n} - \frac{i}{\hbar} E_n \psi_n e^{i\theta_n} e^{i\gamma_n} + i \frac{d\gamma_n}{dt} \psi_n e^{i\theta_n} e^{i\gamma_n} \right] \quad (\text{A.9})$$

$$= [\hat{H} \psi_n] e^{i\theta_n} e^{i\gamma_n} = E_n \psi_n e^{i\theta_n} e^{i\gamma_n} \quad (\text{A.10})$$

and thus

$$\frac{\partial \psi_n}{\partial t} + i\psi_n \frac{d\gamma_n}{dt} = 0. \quad (\text{A.11})$$

Taking the inner product with ψ_n

$$\frac{d\gamma_n}{dt} = i \langle \psi_n | \frac{\partial \psi_n}{\partial t} \rangle. \quad (\text{A.12})$$

Let us assume that the time dependence in the Hamiltonian is given by some (classical) function $R(t)$:

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R} \frac{dR}{dt} \quad \rightarrow \quad \frac{d\gamma_n}{dt} = i \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle \frac{dR}{dt}. \quad (\text{A.13})$$

This can be integrated to give

$$\gamma_n(t) = i \int_0^t \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle \frac{dR}{dt'} dt' = i \int_{R_i}^{R_f} \langle \psi_n | \frac{\partial \psi_n}{\partial R} \rangle dR. \quad (\text{A.14})$$

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

$$\frac{\partial \psi_n}{\partial t} = \frac{\partial \psi_n}{\partial R_1} \frac{dR_1}{dt} + \frac{\partial \psi_n}{\partial R_2} \frac{dR_2}{dt} + \dots + \frac{\partial \psi_n}{\partial R_N} \frac{dR_N}{dt} \quad (\text{A.15})$$

$$= (\nabla_R \psi_n) \cdot \frac{d\vec{R}}{dt}. \quad (\text{A.16})$$

This can be again integrated to give

$$\gamma_n(t) = i \int_{\vec{R}_i}^{\vec{R}_f} \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}. \quad (\text{A.17})$$

If the Hamiltonian is cyclic with period T

$$\gamma_n(T) = i \oint \langle \psi_n | \nabla_R \psi_n \rangle \cdot d\vec{R}. \quad (\text{A.18})$$

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

$$\theta_n(T) = -\frac{1}{\hbar} \int_0^T E_n(t') dt' \quad (\text{A.19})$$

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

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](https://doi.org/10.1103/PhysRevLett.100.177201) (cited on page 84).