Advanced Quantum Mechanics

Tian Lan

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Contents

1 Fundamentals **3**
- 1.1 What is quantum mechanics about, and not about . . . 3
- 1.2 Review: Linear algebra . . . 4
- 1.3 Postulates of quantum mechanics . . . 9
- 1.4 Density operator . . . 11
- 1.5 Commutator and uncertainty relation . . . 11
- 1.6 Position and momentum . . . 12

2 Quantum Dynamics **18**
- 2.1 Evolution operator . . . 18
- 2.2 Dynamical pictures . . . 21
  - 2.2.1 Schrodinger picture, the lab frame as reference . . . 22
  - 2.2.2 Heisenberg picture, the center of mass frame as reference 22
  - 2.2.3 Interaction picture . . . 22
- 2.3 Path integral . . . 23

3 Harmonic Oscillator **26**
- 3.1 Operator method . . . 27
- 3.2 Path integral method . . . 32

4 Symmetry and Conserved Quantities **36**
- 4.1 Space-time translation, energy and momentum . . . 38
- 4.2 Rotation and angular momentum . . . 40
- 4.3 Group and representation . . . 47

5 Many-body Theory **53**
- 5.1 Composite system and tensor product . . . 53
- 5.2 An introductory many-body example . . . 58
- 5.3 Identical particle . . . 60
- 5.4 Field operator . . . 62
- 5.5 Many-body wavefunction . . . 69

6 Perturbation and Scattering Theory **74**
6.1 Non-degenerate perturbation theory 74
6.2 Effective Hamiltonian 77
6.3 Scattering theory 80

Chapter 1

Fundamentals

1.1 What is quantum mechanics about, and not about

Quantum mechanics is a *quantitative description* of the microscopic world. On one hand, everything must finally relate to observables as outcomes of various measurements; on the other hand, the quantitative requirement means mathematics must be involved. At the very basic level, quantum mechanics relates objects in the real world to objects in the mathematical world, and has its own names for these relations, i.e., the postulates:

- The *states* of a physical system form a *Hilbert space*.
- An *observable* corresponds to an *Hermitian operator*.

These two postulates contain more information than they seem to, because Hilbert space and Hermitian operators are very compact mathematical terms with a list of definitions and properties. We will expand on these details in the next section. Besides, the first two postulates do not relate to measurements directly; the third puts them on concrete ground:

- Measurements of an observable O on a state $|\psi\rangle$ are controlled by the *spectrum*, or *eigensystem* of O, in a probabilistic manner:
  - The possible outcomes are the eigenvalues of O.
  - If the outcome is λ, the state becomes a corresponding eigenstate $P_\lambda|\psi\rangle$, where P_λ is the orthogonal projection onto the eigensubspace of λ.
  - The (relative) probability for the outcome to be λ is $\langle\psi|P_\lambda|\psi\rangle$.

Again, we postpone the mathematical details to the following section.

Certainly we also need to postulate the dynamics, i.e., how the system evolves with time. There are several equivalent formulations that we are going to discuss in detail in the next chapter.

Note that these postulates say nothing about specific physical systems. To apply them to a given system, we need to

- Identify the Hilbert space of quantum states;
- Identify of Hermitian operators of observables;
- Identify the dynamics.

Then the physical problem is translated into a mathematical problem. These procedures need to be done in a case by case manner. However, some principles may help. One is the *quantization*, that is, translating the pictures known in classical physics into quantum pictures. One is *symmetry*, to which we will devote a whole chapter.

The next thing is to solve the mathematical problems. Several solving methods will be introduced. But be warned that it is the spirits behind the method, rather than the techniques, that really matter. It is more important to know to which situations the methods apply, and why they do, so that when you encounter new problems, you know what to do and where to find the technical details. However, it is very likely that you will have to invent new methods for new problems.

Beginners may get puzzled by the non-intuitive nature of quantum mechanics. Indeed, the "clean postulates" directly connect observables which can be measured in the real world to the quantities which can be computed in the mathematical world; these "clean postulates" are all we really need, and all that quantum mechanics is about. The extra things, such as intuitive pictures and philosophical interpretations, may or may not help our understanding; unless they can be put down to earth, relating to some measurements in experiments, they make no real difference. It is your freedom to choose what picture or philosophy you believe in; however, probably the most easy way is to "shut up and calculate."

1.2 Review: Linear algebra

A **complex vector space** is a set V whose elements called vectors, equipped with two operations:

- Addition: for any two vectors α and β there is a third vector $\alpha + \beta$.
- Scalar multiplication: for complex number c and vector α, there is a vector $c\alpha$.

satisfying the following eight axioms

1. Associativity of addition: $\alpha + (\beta + \gamma) = (\alpha + \beta) + \gamma$.
2. Commutativity of addition: $\alpha + \beta = \beta + \alpha$.

3. Identity element of addition: There exists an element $\mathbf{0} \in V$, called the zero vector, such that $\alpha + \mathbf{0} = \alpha$ for all $\alpha \in V$.

4. Inverse elements of addition: For every $\alpha \in V$, there exists a vector $-\alpha$ such that $\alpha + (-\alpha) = \mathbf{0}$.

5. Associativity of scalar multiplication: $c_1(c_2\alpha) = (c_1c_2)\alpha$.

6. Identity element of scalar multiplication: $1\alpha = \alpha$.

7. Distributivity of scalar multiplication with respect to vector addition: $c(\alpha + \beta) = c\alpha + c\beta$.

8. Distributivity of scalar multiplication with respect to number addition: $(c_1 + c_2)\alpha = c_1\alpha + c_2\alpha$.

Problem 1.2.1. Verify the properties

1. The zero vector is unique.

2. For any vector α, $0\alpha = \mathbf{0}$.

3. For any number c, $c\mathbf{0} = \mathbf{0}$.

4. The additive inverse $-\alpha$ of α is unique and $-\alpha = (-1)\alpha$.

A linear map, or **operator**, between two vector spaces V and W is a function $f : V \to W$ that preserves addition $f(\alpha + \beta) = f(\alpha) + f(\beta)$ and scalar multiplication $f(c\alpha) = cf(\alpha)$, or equivalently, preserves linear combinations: $f(c_1\alpha + c_2\beta) = c_1f(\alpha) + c_2f(\beta)$. It is more common to denote operators by capital letters $A, B, O, U, \ldots$, and the image of vector α under operator A by $A\alpha$. All the operators from V to W again form a vector space, with addition $(A + B)\alpha = A\alpha + B\alpha$ and scalar multiplication $(cA)\alpha = c(A\alpha)$.

Problem 1.2.2. Verify that the eight axioms of vector space are satisfied by the operators with the above addition and scalar multiplication.

A **basis** of vector space V is a subset of vectors $\{\beta_i\} \subset V$ such that any vector $\gamma \in V$ can be represented by a unique linear combination of β_i,

$$\gamma = c_1\beta_1 + c_2\beta_2 + \cdots + c_n\beta_n.$$

The number of vectors in the basis $\{\beta_i\}$ (or the cardinality if it is an infinite set) is called the **dimension** of the vector space.

The complex numbers $\mathbb{C}$ can be viewed as a one-dimensional vector space. It is easy to see that a vector α in V corresponds to an operator $|\alpha\rangle : \mathbb{C} \to V,\ c \mapsto c\alpha$ in a one-to-one manner. In other words, the vector space of operators from $\mathbb{C}$ to V can be canonically identified with V. This is a good way to understand the *ket* notation widely used in quantum mechanics. Immediately we have

$$|A\alpha\rangle = A|\alpha\rangle,$$

where the right-hand side is interpreted as composition of operators.

An **inner product** on a vector space V assigns, to every pair of vectors α, β, a complex number $\langle\beta|\alpha\rangle$, satisfying

- Linearity: $\langle\beta|c_1\alpha_1 + c_2\alpha_2\rangle = c_1\langle\beta|\alpha_1\rangle + c_2\langle\beta|\alpha_2\rangle$.
- Conjugation symmetry: $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$ where * denotes the complex conjugate. Note that this condition implies the antilinearity of the first argument $\langle c_1\beta_1 + c_2\beta_2|\alpha\rangle = c_1^*\langle\beta_1|\alpha\rangle + c_2^*\langle\beta_2|\alpha\rangle$, and that $\langle\alpha|\alpha\rangle$ is a real number.
- Positive definiteness: $\langle\alpha|\alpha\rangle > 0$ if $\alpha \neq 0$.

A vector space equipped with an inner product is called an inner product space. Two vectors α, β are called orthogonal if $\langle\beta|\alpha\rangle = 0$; a basis $\{\beta_i\}$ is called orthonormal if

$$\langle\beta_i|\beta_j\rangle = \delta_{ij} = \begin{cases} 0, i \neq j \\ 1, i = j \end{cases} .$$

The norm of a vector is defined by $|\alpha| = \sqrt{\langle\alpha|\alpha\rangle}$, and the distance between two vectors is $|\alpha - \beta|$. Then we can discuss Cauchy sequence and completeness. A sequence of vectors $\alpha_1, \alpha_2, \alpha_3, \ldots$ is a Cauchy sequence if for any $\epsilon > 0$, there is an integer N such that for any $n, m > N$, $|\alpha_n - \alpha_m| < \epsilon$. An inner product space is called complete, or a **Hilbert space**, if every Cauchy sequence converges to a vector within the space. In a Hilbert space we can safely do calculus, taking limits, derivatives and integrals.

Similar to the *ket*, we may define a *bra* as an operator $\langle\beta| : V \to \mathbb{C}$, using the inner product

$$\begin{aligned} \langle\beta| : V &\to \mathbb{C}, \\ \alpha &\mapsto \langle\beta|\alpha\rangle. \end{aligned}$$

This way, the notation $\langle\beta|\alpha\rangle$ may also be understood as the composition of $|\alpha\rangle : \mathbb{C} \to V$ and $\langle\beta| : V \to \mathbb{C}$, which is an operator $\mathbb{C} \to \mathbb{C}$ and just a complex number. Such operator point of view unifies various bracket notations: for example, $|\alpha\rangle\langle\beta|$ is an operator $V \to \mathbb{C} \to V$; for $A : V \to W$, $\langle\beta|A|\alpha\rangle$ is a number $\mathbb{C} \to V \to W \to \mathbb{C}$, moreover, when α, β runs over a basis, $\langle\beta|A|\alpha\rangle$ is the matrix elements of operator A.

Given an operator $A : V \to W$, its **Hermitian conjugate** is an operator $A^\dagger : W \to V$ such that for any $\alpha \in V,\ \beta \in W$,

$$\langle\beta|A\alpha\rangle = \langle A^\dagger\beta|\alpha\rangle.$$

In other words, $\langle\alpha|A^\dagger|\beta\rangle = \langle\beta|A|\alpha\rangle^*$, the matrix of $A^\dagger$ is the complex conjugate of the transpose of the matrix of A. We have the following properties

- Antilinearity: $(cA)^\dagger = c^*A^\dagger$, $(A + B)^\dagger = A^\dagger + B^\dagger$.
- $(A^\dagger)^\dagger = A$.

- $(AB)^\dagger = B^\dagger A^\dagger$.
- $(|\alpha\rangle)^\dagger = \langle\alpha|$.

An operator $A : V \to V$ is called **Hermitian** if $A^\dagger = A$. An operator $U : V \to W$ is called **unitary** if $U^\dagger U = \mathrm{id}_V := 1$ and $UU^\dagger = \mathrm{id}_W$ where id_V and 1 denotes the identity operator: $\mathrm{id}_V \alpha = \alpha = 1\alpha$. A unitary operator U preserves inner product in the sense that $\langle U\beta|U\alpha\rangle = \langle\beta|\alpha\rangle$. In particular, if $\{\beta_i\}$ is an orthonormal basis, so is $\{U\beta_i\}$.

Fix an orthonormal basis $\{\beta_i\}$ from now on. Any vector α can be uniquely represented in this basis:

$$|\alpha\rangle = \sum_i c_i|\beta_i\rangle.$$

Then, by the orthonormal condition, $\langle\beta_j|\alpha\rangle = c_j$,

$$|\alpha\rangle = \sum_i |\beta_i\rangle\langle\beta_i|\alpha\rangle,$$

thus,

$$\sum_i |\beta_i\rangle\langle\beta_i| = 1,$$

which is sometimes referred to as a resolution of the identity. We can then deduce that for any two orthonormal bases $\{\alpha_i\}$ and $\{\beta_i\}$, $\sum_i |\alpha_i\rangle\langle\beta_i|$ is a unitary operator. Thus a change of (orthonormal) basis is nothing but a unitary operator.

The **trace** of operator $A : V \to V$ is the sum of diagonal matrix elements, $\mathrm{Tr}\, A = \sum_i \langle\beta_i|A|\beta_i\rangle$. It has the property that $\mathrm{Tr}\, AB = \mathrm{Tr}\, BA$, which can be proved by simply inserting the resolution of the identity:

$$\begin{aligned}\mathrm{Tr}\, AB = \sum_i \langle\beta_i|AB|\beta_i\rangle &= \sum_{ij} \langle\beta_i|A|\beta_j\rangle\langle\beta_j|B|\beta_i\rangle \\ &= \sum_{ij} \langle\beta_j|B|\beta_i\rangle\langle\beta_i|A|\beta_j\rangle = \sum_j \langle\beta_j|BA|\beta_j\rangle = \mathrm{Tr}\, BA.\end{aligned}$$

In particular, this property means that the notion of trace is independent of basis choice: for any unitary U, $\sum_i \langle U\beta_i|A|U\beta_i\rangle = \sum_i \langle\beta_i|U^\dagger AU|\beta_i\rangle = \mathrm{Tr}\, U^\dagger AU = \mathrm{Tr}\, AUU^\dagger = \mathrm{Tr}\, A$.

Problem 1.2.3. Prove that $\mathrm{Tr}\, A^\dagger B$ defines an inner product on the vector space of operators.

If a nonzero vector α satisfies $A\alpha = \lambda\alpha, \lambda \in \mathbb{C}$, α is called an **eigenvector** of A, and λ the corresponding **eigenvalue**. If A satisfies $AA^\dagger = A^\dagger A$ (called *normal*, for example when A is Hermitian or unitary), it is possible to choose an orthonormal basis $\{\alpha_i\}$ from the eigenvectors of A, and in such basis, the matrix of A is diagonal: $\langle\alpha_i|A|\alpha_j\rangle = \lambda_i\delta_{ij}$; equivalently, there exists a unitary operator

U such that $U^\dagger AU$ is diagonal. It is possible that several different basis eigenvectors correspond to the same eigenvalue; such eigenvalue is called degenerate. To deal with degenerate and non-degenerate eigenvalues on equal footing, the notion of **eigensubspace** V_λ, namely the subspace formed by all eigenvectors of eigenvalue λ, is convenient. There is a unique **orthogonal projection** operator $P_\lambda : V \to V$ onto the subspace V_λ, satisfying $P_\lambda^2 = P_\lambda,\ P_\lambda^\dagger = P_\lambda$. In terms of the orthonormal basis $\{\alpha_i\}$ with $A\alpha_i = \lambda_i \alpha_i$,

$$P_\lambda = \sum_{\lambda_i = \lambda} |\alpha_i\rangle\langle\alpha_i|.$$

We see

$$1 = \sum_\lambda P_\lambda.$$

The eigenvectors and eigenvalues may be together called the **eigensystem**, or the **spectrum** of operator A, and the above decomposition is called the spectrum decomposition of A.

Problem 1.2.4. Practice your linear algebra skills in the smallest nontrivial Hilbert space V, i.e., $\dim V = 2$:

1. Let Z be an operator $V \to V$, with the properties

   - Hermitian $Z^\dagger = Z$;
   - Zero trace $\operatorname{Tr} Z = 0$;
   - Unitary $ZZ^\dagger = 1$.

   Write down the matrix of Z in its eigen basis.

2. Let X be another Hermitian unitary operator with zero trace, whose matrix elements in the eigen basis of Z are all real and $XZ = -ZX$. Determine X.

3. Let $Y = \mathrm{i}XZ$. Show that Y is again Hermitian unitary with zero trace.

4. Show that Z, X, Y together with the identity operator 1 form an orthogonal basis of the vector space of operators $V \to V$, with respect to the operator inner product $\operatorname{Tr}(A^\dagger B)$.

5. You have rediscovered the Pauli operators via their nice mathematical properties. Another usual notation of Pauli operators is $\sigma_i,\ i = x, y, z$. Verify their commutation relations

   $$[\sigma_i, \sigma_j] := \sigma_i\sigma_j - \sigma_j\sigma_i = \sum_k 2\mathrm{i}\epsilon_{ijk}\sigma_k,$$

   where $\epsilon_{xyz} = \epsilon_{yzx} = \epsilon_{zxy} = -\epsilon_{yxz} = -\epsilon_{xzy} = -\epsilon_{zyx} = 1$ and all other $\epsilon_{ijk} = 0$.

6. Let $H : V \to V$ be a general Hermitian operator. H can be expressed in terms of the basis $1, Z, X, Y$, $H = a + zZ + xX + yY$ with real numbers a, z, x, y. Find the eigensystem of H and explain how the parameters a and $\boldsymbol{r} = (x, y, z)$ are related to the eigen values and eigen vectors. (Hint: use polar coordinates.)

1.3 Postulates of quantum mechanics

We now revisit the postulates while explaining more details.

- The *states* of a physical system form a *Hilbert space*.

  In particular, it means that linear combinations of states is again a state,

  $$|\psi\rangle = a|\alpha\rangle + b|\beta\rangle.$$

  This is the **superposition**. Multiplying a state $|\psi\rangle$ by a nonzero number c gives the same physical state $c|\psi\rangle$, as an overall factor does not affect the outcomes of measurements. In practice, when $\langle\psi|\psi\rangle$ is finite, we may *normalize* the state by taking $\frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}}$. However, for normalized states there is still a freedom of phase factors $\mathrm{e}^{\mathrm{i}\theta}|\psi\rangle$. Nonetheless, sometimes it is convenient to use non-normalized states.

- An *observable* correspond to an *Hermitian operator*.

  A state with definite value of the observable, is an eigenstate of the Hermitian operator with the definite value being the corresponding eigenvalue. The properties of a Hermitian operator guarantee that the statement makes sense:

  - The eigenvalues of an Hermitian operator are *real*.
  - The Hilbert space can be decomposed in terms of the spectrum of a Hermitian operator, according to which we physically identify the Hilbert space and the operator:
    1. Choose any observable;
    2. Collect all states $|\alpha_i\rangle$ with all possible definite values λ_i of the observable;
    3. The Hilbert space is then spanned by $\{|\alpha_i\rangle\}$; it must contain all states that can be measured, and only those states that can be measured;
    4. The corresponding Hermitian operator is $\sum_i \lambda_i |\alpha_i\rangle\langle\alpha_i|$.

- Measurements of an observable O on a state $|\psi\rangle$ are controlled by the *spectrum*, or *eigensystem* of O, in a probabilistic manner:

  - The possible outcomes are the eigenvalues of O.

– If the outcome is λ, the state becomes a corresponding eigenstate $P_\lambda|\psi\rangle$ (non-normalized), where P_λ is the orthogonal projection onto the eigensubspace of λ.

– The (relative) probability for the outcome to be λ is $\langle\psi|P_\lambda|\psi\rangle$.

Easy to see

$$\sum_\lambda \langle\psi|P_\lambda|\psi\rangle = \langle\psi|\sum_\lambda P_\lambda|\psi\rangle = \langle\psi|\psi\rangle.$$

So the normalized probability is

$$\frac{\langle\psi|P_\lambda|\psi\rangle}{\langle\psi|\psi\rangle},$$

which reduces back to $\langle\psi|P_\lambda|\psi\rangle$ for normalized $|\psi\rangle$. The above formula is more general: it applies to non-normalized states; when both $\langle\psi|P_\lambda|\psi\rangle$ and $\langle\psi|\psi\rangle$ are infinite, their ratio could still be finite.

In the case that the eigenvalue λ is non-degenerate, we can simply label the unique normalized eigenstate by the eigenvalue, i.e. $O|\lambda\rangle = \lambda|\lambda\rangle$ and $P_\lambda = |\lambda\rangle\langle\lambda|$. Assume that $|\psi\rangle$ is also normalized, we got the not so general but more commonly used formula: the probability for obtaining λ in a measurement is $|\langle\lambda|\psi\rangle|^2$ and the state just becomes $|\lambda\rangle$ after the measurement.

The expectation value of the observable is

$$\begin{aligned}\langle O\rangle &= \sum_\lambda \lambda \frac{\langle\psi|P_\lambda|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{1}{\langle\psi|\psi\rangle}\langle\psi|\sum_\lambda \lambda P_\lambda|\psi\rangle \\ &= \frac{1}{\langle\psi|\psi\rangle}\langle\psi|\sum_\lambda OP_\lambda|\psi\rangle = \frac{\langle\psi|O|\psi\rangle}{\langle\psi|\psi\rangle}.\end{aligned}$$

Problem 1.3.1. Consider a two-level system and the observable concerned are the Pauli operators Z, X, Y. Choose the orthonormal eigen basis of Z, $Z|0\rangle = |0\rangle, Z|1\rangle = -|1\rangle$.

1. If we measure Z, X, Y on the state $|\psi\rangle = a|0\rangle + b|1\rangle$, what are the possible outcomes and the corresponding probabilities?

2. What are the expectation $\langle Z\rangle, \langle X\rangle, \langle Y\rangle$ of the state $|\psi\rangle = a|0\rangle + b|1\rangle$? Use polar coordinates

   $$\langle Z\rangle = r\cos\theta,\ \langle X\rangle = r\sin\theta\cos\phi,\ \langle Y\rangle = r\sin\theta\sin\phi.$$

   Calculate r and express the state $|\psi\rangle$ (up to a total factor) in terms of θ and ϕ.

3. If we measured Z and got $+1$, then measure Z again, what are the possible outcomes and corresponding probabilities of the second measurement?

4. If we measured Y and got -1, then measure X, what are the possible outcomes and corresponding probabilities of the second measurement?

1.4 Density operator

It becomes clear that a one-dimensional subspace, instead of a vector, really corresponds to a physical state. Note that the quantities arising in the measurements have the form

$$\langle\psi|A|\psi\rangle = \sum_i \langle\psi|A|\alpha_i\rangle\langle\alpha_i|\psi\rangle = \sum_i \langle\alpha_i|\psi\rangle\langle\psi|A|\alpha_i\rangle = \mathrm{Tr}(|\psi\rangle\langle\psi|A).$$

The projection operator $|\psi\rangle\langle\psi|$ on to the subspace is a cleaner description of a state.

More generally, we may consider a **mixed state**

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

where $0 \leq p_i \leq 1$ is the probability for the system to be in state $|\psi_i\rangle\langle\psi_i|$, with $\sum_i p_i = 1$. In the basis independent form: A **density operator** ρ has the following defining properties

- Hermitian: $\rho^\dagger = \rho$;
- Normalized: $\mathrm{Tr}\,\rho = 1$;
- Positive semi-definite: $\forall\alpha,\ \langle\alpha|\rho|\alpha\rangle \geq 0$.

Measuring O on ρ produces outcome λ and resulting state $\frac{P_\lambda \rho P_\lambda}{\mathrm{Tr}(\rho P_\lambda)}$, with probability $\mathrm{Tr}(\rho P_\lambda)$, and the expectation is $\langle O\rangle = \mathrm{Tr}(\rho O)$.

Problem 1.4.1. Show that the above formulas agree with those in the last section for a pure state $\rho = |\psi\rangle\langle\psi|$.

1.5 Commutator and uncertainty relation

An important feature that distinguishes quantum mechanics from classical mechanics is the fact that two observables can be *incompatible*: they can not have definite values simultaneously. Given two observables A, B and a state $|\psi\rangle$, $|\psi\rangle$ having definite values of A and B simultaneously means $|\psi\rangle$ is a simultaneous eigenstate of A and B. A and B are said **compatible** if their common eigenstate can form a complete orthonormal basis, i.e., there exists a basis $\{|\alpha_i\rangle\}$ such that $A = \sum_i a_i|\alpha_i\rangle\langle\alpha_i|$, $B = \sum_i b_i|\alpha_i\rangle\langle\alpha_i|$. It follows that $AB = BA$. Conversely, if $AB = BA$, consider an eigensubspace V_λ of A. $\forall|\alpha\rangle \in V_\lambda$, $AB|\alpha\rangle = BA|\alpha\rangle = \lambda B|\alpha\rangle$, which means that $B|\alpha\rangle \in V_\lambda$, the action of B restricts in the eigensubspaces of A. Further doing spectrum decomposition of these restrictions leads to a basis that is simultaneous eigenstates of A and B. Thus equivalently, two observables A, B are compatible if they commute $AB = BA$.

It is natural to expect that the **commutator**

$$[A, B] := AB - BA,$$

measures the incompatibility of A and B. Given any state $|\psi\rangle$, let $\Delta A = A - \langle\psi|A|\psi\rangle$, $\Delta B = B - \langle\psi|B|\psi\rangle$. Applying the Cauchy–Schwarz inequality leads to

$$\langle\Delta A\psi|\Delta A\psi\rangle\langle\Delta B\psi|\Delta B\psi\rangle \geq \big|\langle\Delta A\psi|\Delta B\psi\rangle\big|^2.$$

We may also prove the inequality in a more fundamental way, by expanding the left-hand side of the following inequality (ψ omitted)

$$\left((|\Delta A\rangle\langle\Delta B|\Delta B\rangle - |\Delta B\rangle\langle\Delta B|\Delta A\rangle)^\dagger (|\Delta A\rangle\langle\Delta B|\Delta B\rangle - |\Delta B\rangle\langle\Delta B|\Delta A\rangle)\right) \geq 0.$$

Thus the **variances** $\langle(\Delta A)^2\rangle$, $\langle(\Delta B)^2\rangle$ satisfy

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \big|\langle\Delta A\Delta B\rangle\big|^2.$$

Now examine the imaginary part of $\langle\Delta A\Delta B\rangle$ in the right-hand side

$$\begin{aligned}
\mathrm{Im}\langle\Delta A\Delta B\rangle &= \frac{1}{2\mathrm{i}}\left(\langle\Delta A\Delta B\rangle - \langle\Delta A\Delta B\rangle^*\right) \\
&= \frac{1}{2\mathrm{i}}\left(\langle\Delta A\Delta B\rangle - \langle\Delta B\Delta A\rangle\right) \\
&= \frac{1}{2\mathrm{i}}\langle[\Delta A, \Delta B]\rangle = \frac{1}{2\mathrm{i}}\langle[A, B]\rangle.
\end{aligned}$$

It follows that

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}\big|\langle[A, B]\rangle\big|^2,$$

the famous uncertainty relation.

Problem 1.5.1. Determine the condition for minimal uncertainty (when the equality holds).

Problem 1.5.2. Verify the properties of the commutator

$$\begin{gathered}
[A, B] = -[B, A], \\
[A, B + C] = [A, B] + [A, C], \\
[A, BC] = [A, B]C + B[A, C], \\
[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0.
\end{gathered}$$

The last one is known as the Jacobi identity.

1.6 Position and momentum

Now consider a quantum particle moving in 1-dimensional space, with no other internal degrees of freedom. An observable of the particle is its position, corresponding to an operator $\hat{x}$, by which we can also identify the Hilbert space, spanned by $|x\rangle$, the eigenstates of $\hat{x}$, $\hat{x}|x\rangle = x|x\rangle$.

In principle the total Hilbert space only decomposes to the eigensubspaces V_x. Here we assume no observables to distinguish states inside V_x. By the principle that the Hilbert space should not contain things that can not be measured, we have to say that V_x is one-dimensional.

A small difference from what we have learned is that the eigenvalues of $\hat{x}$ form a continuous spectrum. To deal with the continuous case rigorously, we need the mathematics of *functional analysis*. However, that is essentially still linear algebra; we will be good with most technical manipulations as long as we obey several simple rules for the analogy between discrete and continuous cases.

The first rule is to replace discrete summation by integral. Thus the spectrum decomposition of $\hat{x}$ writes

$$1 = \int_{-\infty}^{+\infty} \mathrm{d}x \, |x\rangle\langle x|.$$

Given a state

$$|\psi\rangle = \int \mathrm{d}x \, |x\rangle\langle x|\psi\rangle,$$

the coefficient $\langle x|\psi\rangle$ is called the **wavefunction**, and often written as $\psi(x)$; it contains all the information of the state $|\psi\rangle$. The inner product in terms of wavefunctions is

$$\langle\phi|\psi\rangle = \int \mathrm{d}x \; \phi(x)^* \psi(x).$$

An operator A maps the function $\langle x|\psi\rangle$ to a new one $\langle x|A|\psi\rangle$. Inserting the resolution of identity

$$A\psi(x) = \int \mathrm{d}y \, \langle x|A|y\rangle\psi(y),$$

which has the form of *integral transform* with $\langle x|A|y\rangle$ being the *kernel function*. These are in analogy with matrix multiplication and matrix elements in the discrete case. Interestingly, even if the linear map $\psi(x) \mapsto A\psi(x)$ is well defined, the kernel function $\langle x|A|y\rangle$ may not be a usual function. To name an important example, take A to be the identity operator 1, we have

$$\int \mathrm{d}y \, \langle x|y\rangle f(y) = f(x), \; \forall f.$$

Make a change of variables $y = x + u$, $F(u) = f(x + u)$.

$$\int \mathrm{d}u \, \langle x|x + u\rangle F(u) = F(0),$$

which holds for any x and F. We conclude that $\langle x|y\rangle$ depends on only the difference $y - x$; it worths a name

$$\langle x|y\rangle = \delta(x - y),$$

the **Dirac delta function** $\delta(x)$ with defining property

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

If you examine the value of $\delta(x)$ per point, you find

$$\delta(0) = +\infty,\ \delta(x) = 0,\ \forall x \neq 0.$$

So it is not a function in the usual sense; it is a **distribution** or **generalized function**. Strictly speaking, at this stage we are already beyond the usual notion of Hilbert space, because the inner product $\langle x|y\rangle$ is no longer a usual number. One way to put the above onto concrete ground is to note that there exists a sequence of functions $\{\delta_\epsilon(x)\}$ to approximate $\delta(x)$, in the sense that

$$\lim_{\epsilon\to 0^+} \int \mathrm{d}x\, \delta_\epsilon(x) f(x) = f(0),\ \forall f.$$

This justifies the formal integral notation of the "limiting function" $\delta(x)$. For example

$$\delta_\epsilon(x) = \frac{\mathrm{e}^{-x^2/\epsilon}}{\sqrt{\epsilon\pi}}.$$

Of course such sequence is not unique; any sequence with the properties

$$\begin{cases} \int_a^b \mathrm{d}x\, \delta_\epsilon(x) \to 0,\ (0 \notin (a,b)) \\ \int_a^b \mathrm{d}x\, \delta_\epsilon(x) \to 1,\ (0 \in (a,b)), \end{cases}$$

as $\epsilon \to 0^+$ could do the job. We can manipulate (for example, take derivatives, change variables, ...) the Dirac delta function as if it is a usual function, by manipulating an approximating sequence of functions and then taking the limit. We will also deal with other generalized functions in such manner in the future.

Problem 1.6.1. To understand why the properties

$$\begin{cases} \int_a^b \mathrm{d}x\, \delta_\epsilon(x) \to 0,\ (0 \notin (a,b)) \\ \int_{-\infty}^{+\infty} \mathrm{d}x\, \delta_\epsilon(x) \to 1, \end{cases}$$

as $\epsilon \to 0^+$ are enough for the delta function, check the step function $\theta(x)$ defined by

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0. \end{cases}$$

Show that

$$\theta(x) = \int_{-\infty}^{x} \delta(y)\mathrm{d}y\,.$$

In other words we may formally view the delta function as the derivative of the step function. Use integration by part to compute

$$\int_a^b f(x)\delta(x)\mathrm{d}x\ = \int_a^b f(x)\mathrm{d}\theta(x)\,.$$

Discuss the three cases $a < b < 0$, $a < 0 < b$, and $0 < a < b$.

Recall the **Fourier transform**

$$F(\xi) = \int \mathrm{d}x\, f(x) \mathrm{e}^{-2\pi \mathrm{i} \xi x},$$

whose inverse is

$$f(x) = \int \mathrm{d}\xi\, F(\xi) \mathrm{e}^{2\pi \mathrm{i} \xi x}.$$

Putting them together

$$f(x) = \int \mathrm{d}\xi \left(\int \mathrm{d}y\, f(y) \mathrm{e}^{-2\pi \mathrm{i} \xi y} \right) \mathrm{e}^{2\pi \mathrm{i} \xi x} = \int \mathrm{d}y \left(\int \mathrm{d}\xi\, \mathrm{e}^{2\pi \mathrm{i} \xi (x-y)} \right) f(y).$$

We conclude that

$$\delta(x) = \int \mathrm{d}\xi\, \mathrm{e}^{2\pi \mathrm{i} \xi x} = \frac{1}{2\pi} \int \mathrm{d}k\, \mathrm{e}^{\mathrm{i} k x},$$

which is a very useful representation of the delta function.

Next we want to identify the momentum operator $\hat{p}$. In terms of its own eigenstates, we should have, similar to position case, that the Hilbert space is spanned by $|p\rangle$ and $1 = \int \mathrm{d}p\, |p\rangle\langle p|$, $\langle p_1 | p_2 \rangle = \delta(p_1 - p_2)$. So the question becomes to identify $\langle x | p \rangle$, or equivalently, to express $\hat{p}$ in terms of the position basis $|x\rangle$. In this section we solve the question by assuming the **canonical commutation relation**. We will revisit this problem using the symmetry point of view in the future.

Writing down the canonical commutation relation is a key step in the **canonical quantization** which is a procedure to find the quantum analog of a classical system, suggested by Paul Dirac in 1925. The basic idea is to replace classical variables by quantum operators, while replacing the Poisson brackets by commutators

$$\{x, p\}_{\text{Poisson}} \mapsto \frac{1}{\mathrm{i}\hbar} [\hat{x}, \hat{p}].$$

As of the dynamics, the quantization procedure will be discussed later.

Now we start with the commutator

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar,$$

and derive the representation of $\hat{p}$ in the position basis. We will use a small additional assumption that if the wavefunction $\langle x | \psi \rangle$ is a constant, $|\psi\rangle$ is an eigenstate of $\hat{p}$ with eigenvalue 0. Physically it means that if $|\psi\rangle$ is distributed equally all over the space, then $|\psi\rangle$ is static, not moving at all and has zero momentum. Denote by $|\varphi_0\rangle = \int \mathrm{d}x\, |x\rangle$ one of such states. Given a function of x, $f(x)$, we define the operator $f(\hat{x})$ by the formal Taylor expansion

$$f(\hat{x}) = \sum_n \frac{f^{(n)}(0)}{n!} \hat{x}^n.$$

Problem 1.6.2. When the function is not good enough (can not be expanded as a power series), but the operator A can be diagonalized, $A = \sum_i |\alpha_i\rangle\lambda_i\langle\alpha_i|$, we can still define the operator function

$$f(A) = \sum_i f(\lambda_i)|\alpha_i\rangle\langle\alpha_i|.$$

Prove that the two definitions are equivalent when they both apply.

Then we can verify that

$$\langle x|\psi(\hat{x})|\varphi_0\rangle = \int \mathrm{d}y\, \psi(y)\langle x|y\rangle = \psi(x).$$

Thus, we may express any state $|\psi\rangle$ by

$$|\psi\rangle = \psi(\hat{x})|\varphi_0\rangle.$$

The commutator has the following property

$$[A, BC] = [A, B]C + B[A, C].$$

In other words, $[A, -]$ satisfies a similar algebraic relation as a differential operator when applying to a product, except that one needs to be careful on the order of operators. We immediately have

$$[A, B^n] = \sum_{i=0}^{n-1} B^i[A, B]B^{n-1-i}.$$

Further if $[B, [A, B]] = 0$,

$$[A, B^n] = nB^{n-1}[A, B] = [A, B]\frac{\partial B^n}{\partial B},\ [A, f(B)] = [A, B]\frac{\partial f(B)}{\partial B}.$$

We call it the differential property of the commutator, which will be used quite often again in this course, so take a note of it. Thus it is also true that

$$[f(\hat{x}), \hat{p}] = \mathrm{i}\hbar\frac{\partial f(\hat{x})}{\partial \hat{x}}.$$

Therefore,

$$\begin{aligned}
\langle x|\hat{p}|\psi\rangle &= \langle x|\hat{p}\psi(\hat{x})|\varphi_0\rangle \\
&= \langle x|\psi(\hat{x})\hat{p} - \mathrm{i}\hbar\frac{\partial\psi(\hat{x})}{\partial\hat{x}}|\varphi_0\rangle \\
&= -\mathrm{i}\hbar\langle x|\frac{\partial\psi(\hat{x})}{\partial\hat{x}}|\varphi_0\rangle \\
&= -\mathrm{i}\hbar\frac{\partial\psi(x)}{\partial x} = -\mathrm{i}\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle,
\end{aligned}$$

which is the representation of $\hat{p}$ in the position basis. Then we can solve for the momentum eigenstates

$$p\langle x|p\rangle = \langle x|\hat{p}|p\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\langle x|p\rangle.$$

The solution is

$$\langle x|p\rangle = C\mathrm{e}^{\mathrm{i}px/\hbar}.$$

To obtain the constant C, consider the normalization condition

$$\delta(x-y) = \langle x|y\rangle = \int \mathrm{d}p\,\langle x|p\rangle\langle p|y\rangle = \int \mathrm{d}p\,|C|^2\mathrm{e}^{\mathrm{i}p(x-y)/\hbar} = 2\pi\hbar|C|^2\delta(x-y).$$

Thus we take $C = 1/\sqrt{2\pi\hbar}$, and

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

It is the basis function of Fourier transform. We learned the key message that in quantum mechanics position and momentum are Fourier transforms of each other.

Problem 1.6.3. Derive the commutation relation

$$[\hat{x},\hat{p}] = \mathrm{i}\hbar,$$

and $\int \mathrm{d}x\,\hat{p}|x\rangle = 0$ from the Fourier transform relation

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

It follows that the following three definitions of $\hat{p}$ operator are equivalent

- $\begin{cases}[\hat{x},\hat{p}] = \mathrm{i}\hbar,\\ \int \mathrm{d}x\,\hat{p}|x\rangle = 0,\end{cases}$
- $\langle x|\hat{p}|\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle,$
- $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar}.$

Chapter 2

Quantum Dynamics

2.1 Evolution operator

Under the assumption that the Hilbert space included all the relevant physical entities, processes and observables, any quantum time evolution is essentially a *rotation* in the Hilbert space. Both the states and the observable operators could evolve with time. Pick a zero point of time, when the state is $|\psi\rangle$ and observable is O. For the state $|\psi(t)\rangle$ at time t, we take the convention

$$|\psi(t)\rangle = U_\psi(t)|\psi\rangle.$$

For the observable $O(t)$ at time t, we take the convention that its eigenstate $|\alpha\rangle$ evolves as

$$|\alpha, t\rangle = U_O^\dagger(t)|\alpha\rangle,$$

and the operator evolves as

$$O(t) = U_O^\dagger(t) O U_O(t).$$

$U_\psi(t), U_O(t)$ are unitary operators with $U_\psi(0) = U_O(0) = 1$. The reason to reverse the convention is that when measurements of O is concerned, we need to consider $\langle\alpha, t|\psi(t)\rangle$, or $\langle\psi(t)|O(t)|\psi(t)\rangle$, whose evolution is governed by the total "relative" evolution $U(t) = U_O(t)U_\psi(t)$. It is convenient to introduce notations for the evolution from time t to time s

$$U_\psi(s,t) = U_\psi(s)U_\psi^\dagger(t), \quad U_O(s,t) = U_O^\dagger(t)U_O(s).$$

However, since operators are generally non-commutative,

$$U(s) = U_O(s)U_\psi(s) = U_O(t)U_O(s,t)U_\psi(s,t)U_\psi(t),$$

where the evolution occurs neither to the left nor to the right, but *inside*. We have to make a choice in order to define $U(s,t)$. If we want $U(t)$ to follow the same convention as $U_\psi(t)$,

$$U(s,t) = U(s)U^\dagger(t) = U_O(t)\Big(U_O(s,t)U_\psi(s,t)\Big)U_O^\dagger(t), \tag{2.1}$$

where the conjugation by $U_O(t)$ is the price we have to pay when moving the origin of time to t. Then we have the composition relation

$$U(t,u)U(u,s) = U(t,s),$$

and similar for $U_\psi(t,s), U_O(t,s)$.

We are most interested in the total relative evolution $U(t)$ (similar discussion applies to $U_\psi(t)$ and $U_O(t)$). If we know every *infinitesimal* evolution $U(t+\delta t, t)$ we can multiply them together to get the total evolution.

$$U(t+\delta t, t) = 1 + \left.\frac{\partial U(s,t)}{\partial s}\right|_{s=t} \delta t + o(\delta t).$$

By the unitarity of $U(s,t)$, it is easy to show

$$0 = \left.\frac{\partial}{\partial s}\left(U(s,t)U^\dagger(s,t)\right)\right|_{s=t} = \left.\frac{\partial U(s,t)}{\partial s}\right|_{s=t} + \left.\frac{\partial U^\dagger(s,t)}{\partial s}\right|_{s=t}.$$

Thus $\left.\frac{\partial U(s,t)}{\partial s}\right|_{s=t}$ is *skew-Hermitian*, whose eigenvalues are purely imaginary. We define the **Hamiltonian** operator

$$H(t) := \mathrm{i}\hbar \left.\frac{\partial U(s,t)}{\partial s}\right|_{s=t},$$

which is Hermitian and has the dimension of energy. The Hamiltonian is the **generator** of the evolution operator, in other words, generator of the time translation. Note that $H(t)$ is *not* the Hamiltonian operator evolved to time t. It is logically misleading to speak of the time evolution of time evolution operator; for the same reason we also avoid speaking of the time evolution of Hamiltonian operator, though many textbooks discussed this and obtained seemingly consistent result.

We obtain the partial differential equation

$$\left.\frac{\partial U(s)}{\partial s}\right|_{s=t} = \left.\frac{\partial U(s,t)U(t)}{\partial s}\right|_{s=t} = \left.\frac{\partial U(s,t)}{\partial s}\right|_{s=t} U(t),$$

namely

$$\mathrm{i}\hbar \frac{\partial U(t)}{\partial t} = H(t)U(t).$$

To see that the Hamiltonian indeed physically represents the energy operator, recall that if a system is time-translation invariant, then its energy is conserved. Now assume the evolution operator is time-translation invariant, $U(s,t) = U(s-t,0) = U(s-t)$, we conclude

$$H = \mathrm{i}\hbar \left.\frac{\partial U(t)}{\partial t}\right|_{t=0},$$

is independent of time. It is then easy to obtain the solution to the PDE

$$U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}.$$

H and $U(t)$ has common eigenstates. The evolution of an eigenstate with definite value of H only picks up a total phase factor. The expectation value $\langle H\rangle$ is a constant. Indeed, H corresponds to energy.

For a time dependant $H(t)$, we can use the philosophy of integral, and think $H(t)$ as constant in a small enough time interval δt

$$U(t+\delta t,t)\approx \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(\tilde{t})\delta t},$$

where $\tilde{t}\in[t,t+\delta t]$. Then we multiply them together while taking the limit $\delta t\to 0$,

$$\mathcal{T}\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t\, H(t)}\right):=\lim_{\substack{\delta t\to 0\\ n\to\infty}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(\tilde{t}_n)\delta t}\cdots \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H(\tilde{t}_1)\delta t}=U(t),$$

where $\tilde{t}_n>\cdots>\tilde{t}_1$ are in each small interval. Note that the notation

$$\mathcal{T}\left(\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t\, H(t)}\right)$$

should be understood as a whole, the *time-ordered multiplicative integral*. It does not mean to take first an additive integral $-\int_0^t \mathrm{d}t\,\mathrm{i}H(t)/\hbar$ and then the exponential; the order of operations matter here, since when A,B do not commute, $\mathrm{e}^{A+B}\neq \mathrm{e}^A\mathrm{e}^B\neq \mathrm{e}^B\mathrm{e}^A$.

We may similarly define the Hamiltonians $H_\psi(t), H_O(t)$

$$H_\psi(t)=\mathrm{i}\hbar\frac{\partial U_\psi(s,t)}{\partial s}\bigg|_{s=t},\quad H_O(t)=\mathrm{i}\hbar\frac{\partial U_O(s,t)}{\partial s}\bigg|_{s=t}.$$

Equivalently,

$$\mathrm{i}\hbar\frac{\partial U_\psi(t)}{\partial t}=H_\psi(t)U_\psi(t),\quad \mathrm{i}\hbar\frac{\partial U_O(t)}{\partial t}=U_O(t)H_O(t),$$

and by differentiating $U(t)=U_O(t)U_\psi(t)$ or eq.(2.1), we find

$$U_O^\dagger(t)H(t)U_O(t)=H_\psi(t)+H_O(t).$$

The PDE for the states and operators read

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle=H_\psi(t)|\psi(t)\rangle,$$

$$\frac{\partial}{\partial t}O(t)=\frac{\mathrm{i}}{\hbar}[H_O(t),O(t)].$$

Problem 2.1.1. We have assumed in the above that there are only quantum evolutions for the operator $O(t)$. In practice it is often convenient to consider an operator A_t with time dependence not from quantum evolutions (for example $A_t=Of(t)$ for some function f). In this case, the total evolved operator is

$$A_t(t)=U_O^\dagger(t)A_tU_O(t).$$

Derive the PDE obeyed by $A_t(t)$.

To describe a quantum system, it is thus a key step to identify the Hamiltonian operator. When the system has classical limit or classical analog, in the **canonical quantization** one simply takes the classical Hamiltonian, replacing classical variables by quantum operators satisfying the canonical commutation relation, to produce the quantum Hamiltonian operator. For example, for a particle moving in one-dimensional potential $V(x)$ whose classical Hamiltonian is

$$H = \frac{p^2}{2m} + V(x),$$

the corresponding quantum Hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

Problem 2.1.2. Suppose that we have a classical system with Hamiltonian

$$H = \sum_{a,b=0}^{\infty} C_{a,b} x^a p^b = \sum_{a,b=0}^{\infty} C_{a,b} p^b x^a$$

where $C_{a,b}$ are some constants. Since $\hat{x}$ and $\hat{p}$ do not commute, there is in general ambiguity (the order of operators) to perform canonical quantization. Compute the difference between different orders of operators and

1. Show that the terms with $a + b < 4$ does not suffer from such ambiguity.
2. Show that the ambiguity is acceptable for terms with $a + b = 4$, in the sense that it only shifts the energy zero point.
3. Show that the ambiguity is no longer acceptable for terms with $a + b > 4$.

(Hint: Remember to make your Hamiltonian operator Hermitian.)

2.2 Dynamical pictures

The dynamical pictures are equivalent ways to describe quantum dynamics; different pictures are quantum analogs of different reference of frames in classical physics. The picture we discussed in the last section is the most general one: both the states and observable operators evolve. In this section, we discuss three most commonly used dynamical pictures. The convention is as before: observable operators (the lab frame) are governed by the evolution operator $U_O(t)$. The states (the center of mass frame) are governed by the evolution operator $U_\psi(t)$. Measurements are only affected by the relative evolution $U(t) = U_O(t)U_\psi(t)$. In the following three pictures, the Hamiltonian corresponding to the relative evolution $H(t) = \mathrm{i}\hbar \frac{\partial U(s,t)}{\partial s}\Big|_{s=t}$ are taken to be the same, which guarantees the equivalence of the three pictures.

2.2.1 Schrodinger picture, the lab frame as reference

- Operators stay still, $U_O(t) = 1$, $O(t) = O(0) = O$.
- States evolve, $U_\psi(t) = U(t)$, $|\psi(t)\rangle = U(t)|\psi(0)\rangle$.
- Schrodinger equation

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

2.2.2 Heisenberg picture, the center of mass frame as reference

- States stay still, $U_\psi(t) = 1$, $|\psi(t)\rangle = |\psi(0)\rangle$.
- Operators evolve, $U_O(t) = U(t)$, $O(t) = U^\dagger(t)OU(t)$, and eigenstates $|\alpha, t\rangle = U^\dagger(t)|\alpha, 0\rangle$.
- Heisenberg equation

$$\frac{\partial}{\partial t}O(t) = \frac{\mathrm{i}}{\hbar}[U^\dagger(t)H(t)U(t), O(t)].$$

  Note that $[U^\dagger(t)H(t)U(t), -]$ is a linear operator acting on the vector space of operators. It has the same form as the Schrodinger equation: the time derivative of a vector equals to a linear operator acting on the same vector. Thus we can immediately write down the solution

$$O(t) = \mathcal{T}\left(\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t\,[U^\dagger(t)H(t)U(t),-]}\right)O.$$

  When the Hamiltonian does not depend on time explicitly, it reduces to

$$O(t) = \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}[H,-]}O = O + \frac{\mathrm{i}t}{\hbar}[H, O] + \frac{(\mathrm{i}t)^2}{2!\hbar^2}[H, [H, O]] + \ldots$$

2.2.3 Interaction picture

- Assume that the Hamiltonian can be split into two parts

$$H(t) = H_f + H_i(t),$$

  where H_f is the time-independent *free* part which we understand relatively well, and $H_i(t)$ is the *interacting* part.
- Operators evolve as $U_O(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_f t}$.
- States evolve as $U_\psi(t) = U_O(t)^\dagger U(t) = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H_f t}U(t)$.
- Schwinger-Tomonaga equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \mathrm{e}^{\frac{\mathrm{i}}{\hbar}H_f t}H_i(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H_f t}|\psi(t)\rangle.$$

Problem 2.2.1. Although we have been talking about time evolution operators, the techniques used are in fact quite universal in quantum mechanics, when the exponential of operators together with a real parameter is involved. Prove the following famous and useful formulas

1. If $AB = BA$, use the power expansion of exponential function to prove that
$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{A+B}.$$
In particular $\mathrm{e}^{-A}\mathrm{e}^{A} = \mathrm{e}^{0} = 1$.

2. The Hadamard formula
$$\begin{aligned}\mathrm{e}^{A}B\mathrm{e}^{-A} = \mathrm{e}^{[A,-]}B &= \sum_{n}\frac{1}{n!}[A,-]^{n}B \\ &= B + [A,B] + \frac{1}{2}[A,[A,B]] + \frac{1}{6}[A,[A,[A,B]]] + \cdots .\end{aligned}$$
Similar to the case of the operator evolution, you can consider the differential of $\mathrm{e}^{rA}B\mathrm{e}^{-rA}$ with respect to the real number r, and then set $r = 1$. So we know how the exchange the multiplication order of e^{A} and B, $\mathrm{e}^{A}B = \mathrm{e}^{[A,-]}B\mathrm{e}^{A}$.

3. The special Baker-Campbell-Hausdorff formula, assuming that $[A,B]$ commutes with both A and B,
$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{[A,B]/2}\mathrm{e}^{A+B}.$$
Consider the differential of $\mathrm{e}^{rA}\mathrm{e}^{rB}\mathrm{e}^{-r(A+B)}$ with respect to the real number r, and then set $r = 1$.

2.3 Path integral

Besides the Hamiltonian approach to determining the quantum evolution, another effective approach is using the *path integral*. Put it simply, to obtain the evolution operator $U(T)$, we may insert the resolution of identity at times $0 = t_0 < t_1 < t_2 < \cdots < t_n = T$

$$\begin{aligned}U(T) &= U(t_n,t_{n-1})U(t_n,t_{n-1})\cdots U(t_1,t_0) \\ &= \int \mathrm{d}x_0\cdots\mathrm{d}x_n\,|x_n\rangle\langle x_n|U(t_n,t_{n-1})|x_{n-1}\rangle\langle x_{n-1}|U(t_{n-1},t_{n-2})|x_{n-2}\rangle \\ &\quad \langle x_{n-2}|\cdots|x_{i+1}\rangle\langle x_{i+1}|U(t_{i+1},t_i)|x_i\rangle\langle x_i|\cdots \\ &\quad \cdots|x_1\rangle\langle x_1|U(t_1,t_0)|x_0\rangle\langle x_0|.\end{aligned}$$

Using the basis in the Heisenberg picture $|x,t\rangle = U^{\dagger}(t)|x\rangle$, the matrix elements can be rewritten as
$$\langle x'|U(t',t)|x\rangle = \langle x',t'|x,t\rangle.$$

This quantity is usually referred to as the *propagator*, which is the transition amplitude from spacetime point x, t to x', t'. Thus the matrix elements of the evolution operator as above can be put in a more compact and motivating form

$$\langle x_n|U(T)|x_0\rangle = \langle x_n, T|x_0, 0\rangle = \int \mathrm{d}x_1 \cdots \mathrm{d}x_{n-1} \prod_{i=1}^{n} \langle x_i, t_i|x_{i-1}, t_{i-1}\rangle.$$

Each sequence $(x_0, t_0), (x_1, t_1), \cdots, (x_n, t_n)$ can be viewed as a discrete path and each path is associated with a complex number

$$W[\{x_i, t_i\}] = \prod_{i=1}^{n} \langle x_i, t_i|x_{i-1}, t_{i-1}\rangle.$$

By summing $W[\{x_i, t_i\}]$ over all possible paths one obtains the evolution. This the key idea of path integral.

In practice, we need to further take the continuum limit, $n \to \infty, |t_i - t_{i-1}| \to 0$, such that

- the discrete sequence $\{x_i, t_i\}$ becomes a function $x(t)$ of path;
- $W[x(t)]$ is now a functional (function which takes a function as the input variable) of the path $x(t)$
- the multi-dimensional integration $\int \mathrm{d}x_0 \cdots \mathrm{d}x_n$,
  becomes an infinite-dimensional integration, which is usually denoted by

$$\int \mathcal{D}[x(t)] := \lim_{n\to\infty} \int \mathrm{d}x_0 \cdots \mathrm{d}x_n \,.$$

Now the matrix elements of the evolution operator is

$$\langle x', T|x, 0\rangle = \langle x'|U(T)|x\rangle = \int_{x(0)=x}^{x(T)=x'} \mathcal{D}[x(t)] W[x(t)].$$

It is then intriguing to investigate the form of the functional $W[x(t)]$ associated to the path $x(t)$. To get some intuition, let's evaluate the simplest example, the propagator of a free particle.

$$\begin{aligned}
\langle x'|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}T}|x\rangle &= \int \mathrm{d}p\, \langle x'|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\frac{\hat{p}^2}{2m}T}|p\rangle\langle p|x\rangle \\
&= \int \mathrm{d}p\, \frac{1}{2\pi\hbar} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(\frac{p^2}{2m}T - p(x-x'))} \\
&= \frac{1}{2\pi\hbar} \int \mathrm{d}p\, \mathrm{e}^{-\frac{\mathrm{i}T}{2m\hbar}(p - \frac{m(x-x')}{T})^2 + \frac{\mathrm{i}}{\hbar}\frac{1}{2}m\frac{(x'-x)^2}{T}} \\
&= \sqrt{\frac{m}{\mathrm{i}2\pi\hbar T}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\frac{1}{2}m\frac{(x'-x)^2}{T}}.
\end{aligned}$$

Note that

$$\frac{1}{2}m\frac{(x'-x)^2}{T} = \int_0^T \frac{1}{2}mv^2 \mathrm{d}t\,,$$

is the classical action of the free particle along its classical path ($v = (x'-x)/T$ is a constant). More generally,

$$W[x(t)] = F\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S[x(t)]},$$

where F is a normalization factor (which does not depend on the path) and $S[x(t)]$ is the classical action of the system. It is a usual convention to absorb the normalization factor F into the definition of $\mathcal{D}[x(t)]$ (as the measure of the path), namely

$$\int \mathcal{D}[x(t)] := \lim_{n\to\infty} F \int \mathrm{d}x_0 \cdots \mathrm{d}x_n\,.$$

Thus

$$\langle x', T|x, 0\rangle = \langle x'|U(T)|x\rangle = \int_{x(0)=x}^{x(T)=x'} \mathcal{D}[x(t)]\mathrm{e}^{\frac{\mathrm{i}}{\hbar}S[x(t)]}.$$

Let's check the classical limit ($\hbar \to 0$) to see why the form makes sense. Recall that the classical path is determined by the stationary point of the action

$$\delta S[x(t)] = 0.$$

As $\hbar \to 0$, $\mathrm{e}^{\mathrm{i}S/\hbar}$ will oscillate very violently so that most adjacent paths contribute destructively to the path integral. Only near the stationary point $\delta S[x(t)] = 0$, when we deform the path a little bit, the phase remains almost the same and contribute constructively to the path integral. As a result, in the classical limit, the classical path is singled out, as desired.

Problem 2.3.1. For a one-dimensional potential $V(x)$ and small time interval δt, verify that, to the first order of δt,

$$\langle x'|\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}H\delta t}|x\rangle \sim \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S},$$

where

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}).$$

$$S = L\delta t, \quad L = \frac{1}{2}m\dot{x}^2 - V(x) = \frac{1}{2}m\left(\frac{x'-x}{\delta t}\right)^2 - V(x).$$

(L is the classical *Lagrangian*.)

To conclude, the dynamics of a quantum system is described by the quantum evolution operator, which is determined, either by the Hamiltonian operator, or the action/Lagrangian via path integral. We will show both approaches in the next section for quantum harmonic oscillator.

Chapter 3

Harmonic Oscillator

In this chapter, we will study the quantum harmonic oscillator in detail. We begin by reviewing the canonical quantization procedure. A classical harmonic oscillator is a particle moving in a one-dimensional quadratic potential. The classical Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{1}{2m}\left(p^2 + m^2\omega^2 x^2\right),$$

where m is the mass of the particle, k is the spring constant. x, p are the classical dynamical variables, position and momentum, conjugate to each other. It is more conventional to use the angular frequency $\omega = \sqrt{k/m}$. So a quantum harmonic oscillator has the Hilbert space with the position states $|x\rangle$ being a basis, and Hamiltonian

$$H = \frac{1}{2m}\left(\hat{p}^2 + m^2\omega^2\hat{x}^2\right),$$

where the position and momentum operators $\hat{x}, \hat{p}$ are as we discussed in Section 1.6, satisfying

$$[\hat{x}, \hat{p}] = \mathrm{i}\hbar,\ \hat{x}|x\rangle = x|x\rangle,\ \langle x|\hat{p}|\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial x}\langle x|\psi\rangle.$$

So in the position basis

$$\langle x|H|\psi\rangle = \frac{1}{2m}\left(-\hbar^2\frac{\partial^2}{\partial x^2} + m^2\omega^2 x^2\right)\langle x|\psi\rangle.$$

It is then a straightforward approach to solve the differential equation for the eigen wavefunctions. However, solving differential equations would be the ultimate backup approach; we will introduce a more elegant operator method, first developed by Dirac based on earlier work of M. Born and N. Wiener.

3.1 Operator method

It is a common practice in linear algebra to simplify the problem by forming new linear combinations of vectors or operators. We now explore along this way. First, to make the derivation clear, define

$$P = \frac{\hat{p}}{\sqrt{2m}},\ X = \sqrt{\frac{m}{2}}\omega\hat{x}.$$

We want to find new operators

$$A = \alpha X + \beta P,\ B = \mu X + \nu P,$$

which can simplify the eigenvalue problem

$$H = X^2 + P^2,\ [X, P] = \frac{\mathrm{i}}{2}\hbar\omega.$$

We can write the transformation in matrix form

$$(A, B) = (X, P)\begin{pmatrix}\alpha & \mu\\ \beta & \nu\end{pmatrix}.$$

So the first requirement is that the matrix $T := \begin{pmatrix}\alpha & \mu\\ \beta & \nu\end{pmatrix}$ is invertible so that we can transform back from A, B to X, P. Thus, $\det T = \alpha\nu - \beta\mu \neq 0$, and

$$(X, P) = (A, B)T^{-1},\ T^{-1} = \frac{1}{\det T}\begin{pmatrix}\nu & -\mu\\ -\beta & \alpha\end{pmatrix}.$$

Expand the above

$$X = \frac{1}{\det T}(\nu A - \beta B),\ P = \frac{1}{\det T}(-\mu A + \alpha B),$$

and plug them into the Hamiltonian

$$H = \left(\frac{1}{\det T}\right)^2\Big((\nu^2 + \mu^2)A^2 + (\alpha^2 + \beta^2)B^2 - (\alpha\mu + \beta\nu)(AB + BA)\Big).$$

The commutation relation of A, B is

$$[A, B] = [\alpha X + \beta P, \mu X + \nu P] = (\alpha\nu - \beta\mu)[X, P] = \det T[X, P],$$

just $[X, P]$ times a non-zero constant. Since $H = X^2 + P^2$ can not be easily solved, after the transformation to A, B we want to make the coefficients of the squared terms be zero

$$\alpha^2 + \beta^2 = 0,\ \mu^2 + \nu^2 = 0.$$

So we choose

$$\beta = \mathrm{i}\alpha,\ \nu = -\mathrm{i}\mu.$$

Then $\det T = -2\mathrm{i}\alpha\mu \neq 0$. Plug these back into the Hamiltonian

$$H = \frac{1}{2\alpha\mu}(AB + BA) = \frac{1}{2\alpha\mu}(BA + [A, B] + BA)$$
$$= \frac{1}{\alpha\mu}BA - \mathrm{i}[X, P] = \frac{B}{\mu}\frac{A}{\alpha} + \frac{1}{2}\hbar\omega.$$

Define the *annihilation* operator

$$a := \frac{1}{\sqrt{\hbar\omega}}\frac{A}{\alpha} = \frac{1}{\sqrt{\hbar\omega}}(X + \mathrm{i}P) = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \mathrm{i}\frac{\hat{p}}{\sqrt{2m\hbar\omega}},$$

and its Hermitian conjugate the *creation* operator (the meaning of the names will be clear shortly)

$$a^\dagger = \frac{1}{\sqrt{\hbar\omega}}\frac{B}{\mu} = \frac{1}{\sqrt{\hbar\omega}}(X - \mathrm{i}P) = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \mathrm{i}\frac{\hat{p}}{\sqrt{2m\hbar\omega}}.$$

$a, a^\dagger$ together are called the *ladder* operators, with commutation relation

$$[a, a^\dagger] = 1.$$

We now study the properties of the ladder operators to see how they greatly simplify the Hamiltonian

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

1. We call the Hermitian operator

   $$N = a^\dagger a$$

   as the *number* operator. There are the following commutation relations

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

   Suppose that $|\phi_n\rangle$ is an eigenstate of N, $N|\phi_n\rangle = n|\phi_n\rangle$.

   $$Na|\phi_n\rangle = (aN - a)|\phi_n\rangle = (n - 1)a|\phi_n\rangle,$$

   namely if $a|\phi_n\rangle \neq 0$, it is an eigenstate of N with eigenvalue $n - 1$. Similarly,

   $$Na^\dagger|\phi_n\rangle = (a^\dagger N + a^\dagger)|\phi_n\rangle = (n + 1)a^\dagger|\phi_n\rangle,$$

   if $a^\dagger|\phi_n\rangle \neq 0$ it is an eigenstate of N with eigenvalue $n + 1$.

2. $N = a^\dagger a$ is a positive semi-definite operator, namely for any state $|\phi\rangle$, $\langle\phi|N|\phi\rangle = \langle a\phi|a\phi\rangle \geq 0$. Thus the eigenvalues of N must be non-negative. However, each application of a to an eigenstate reduces the eigenvalue by 1; such process has to stop after finite steps. In other words, there must exist a non-zero state $|\psi\rangle$ such that $a|\psi\rangle = 0$ is a zero state vector. $N|\psi\rangle = a^\dagger a|\psi\rangle = 0$, namely, $|\psi\rangle$ is an eigenstate of N with eigenvalue 0. Since $a|\psi\rangle = 0 \Rightarrow N|\psi\rangle = 0$, for an eigenstate $|\phi_n\rangle$ with non-zero eigenvalue it is not possible that $a|\phi_n\rangle = 0$. Therefore, the eigenvalues of N can only be non-negative integers; otherwise, by applying a the eigenvalue will never reach zero thus never stop decreasing, contradiction.

3. How many (linear independent) eigenstates are there with eigenvalue 0? This question can not be answered given only the algebraic properties of a. However, the differential equation

$$\langle x|a|\psi\rangle = \sqrt{\frac{m\omega}{2\hbar}}x\psi(x) + \mathrm{i}\frac{-\mathrm{i}\hbar}{\sqrt{2m\hbar\omega}}\frac{\partial\psi(x)}{\partial x} = 0$$

is easy to solve. The general solution is

$$\psi(x) = C\mathrm{e}^{-\frac{m\omega}{2\hbar}x^2}.$$

It is the ground state of the harmonic oscillator, which is non-degenerate. Denote by $|0\rangle$ the normalized ground state

$$\langle x|0\rangle = \Big(\frac{m\omega}{\pi\hbar}\Big)^{1/4}\mathrm{e}^{-\frac{m\omega}{2\hbar}x^2}.$$

4. By repeated applying $a^\dagger$ to the ground state $|0\rangle$ we obtain the excited eigenstates. We can also prove that all eigenstates can be obtained this way. Let $|\phi_n\rangle$ be an eigenstate with eigenvalue n. $a^n|\phi_n\rangle$ is then a ground state. We have shown that the ground state is non-degenerate, thus there must be a nonzero constant C such that $a^n|\phi_n\rangle = C|0\rangle$. Then we evaluate

$$\begin{aligned}(a^\dagger)^n a^n|\phi_n\rangle &= (a^\dagger)^{n-1}Na^{n-1}|\phi_n\rangle\\ &= 1\times(a^\dagger)^{n-2}Na^{n-2}|\phi_n\rangle\\ &= 1\times 2\times(a^\dagger)^{n-3}Na^{n-3}|\phi_n\rangle\\ &= \cdots = n!|\phi_n\rangle = (a^\dagger)^n C|0\rangle.\end{aligned}$$

Thus, $|\phi_n\rangle = \frac{C}{n!}(a^\dagger)^n|0\rangle$. Now we compute the norm of $(a^\dagger)^n|0\rangle$ to fix normalization. Recall the "differential" property of commutator, $[a,(a^\dagger)^n] = n(a^\dagger)^{n-1}$.

$$\begin{aligned}\langle 0|a^n(a^\dagger)^n|0\rangle &= \langle 0|a^{n-1}a(a^\dagger)^n|0\rangle\\ &= \langle 0|a^{n-1}(n(a^\dagger)^{n-1} + (a^\dagger)^n a)|0\rangle\\ &= n\langle 0|a^{n-1}(a^\dagger)^{n-1}|0\rangle = \cdots = n!.\end{aligned}$$

Therefore we can define the *number basis* or *occupation basis*,

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle,$$

which are orthonormal eigenstates

$$N|n\rangle = n|n\rangle,\ \langle m|n\rangle = \delta_{mn}.$$

In this basis

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

Now we have solved the quantum harmonic oscillator whose energy eigenstates are $|n\rangle$ with energy $\hbar\omega(n+1/2)$. Physically, we think that in a harmonic oscillator there is a minimal energy quantum $\hbar\omega$. $a^\dagger$ creates a quantum, a annihilates a quantum and $N = a^\dagger a$ measures the total number of quanta, hence their names. The groundstate $|0\rangle$ is free of quanta, thus also called the vacuum state. The excited state $|n\rangle$ is obtained by creating n quanta from the vacuum.

Passing to position basis, we have

$$\langle x|n\rangle = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\left(\sqrt{\frac{m\omega}{\hbar}}x - \frac{\partial}{\partial(\sqrt{\frac{m\omega}{\hbar}}x)}\right)^n \mathrm{e}^{-\frac{1}{2}(\sqrt{\frac{m\omega}{\hbar}}x)^2}.$$

It is easy to see these wavefunctions have the form of a polynomial times the exponential. The polynomials arising this way are known as the *Hermite polynomials*

$$H_n(x) = \mathrm{e}^{\frac{1}{2}x^2}\left(x - \frac{\partial}{\partial x}\right)^n \mathrm{e}^{-\frac{1}{2}x^2},$$

or equivalently the more standard definition

$$H_n(x) = \mathrm{e}^{x^2}\left(-\frac{\partial}{\partial x}\right)^n \mathrm{e}^{-x^2}.$$

So that the eigen wavefunctions are

$$\langle x|n\rangle = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\mathrm{e}^{-\frac{1}{2}(\sqrt{\frac{m\omega}{\hbar}}x)^2}.$$

Problem 3.1.1. Verify the two definitions of Hermite polynomials are equivalent. (Hint: Use mathematical induction.)

We then briefly discuss the eigenstates of a, also known as the *coherent states*. Similar to the trick we have used when deriving the eigenstates of $\hat{p}$ from the commutation relation, now we have a state $|0\rangle$ such that $a|0\rangle = 0$, thus for any function f, the action of a on the state $f(a^\dagger)|0\rangle$ is clear

$$af(a^\dagger)|0\rangle = (f'(a^\dagger) + f(a^\dagger)a)|0\rangle = f'(a^\dagger)|0\rangle.$$

Thus we immediately obtain that the eigenstate of a should be given by the exponential function

$$|\alpha\rangle = \frac{\mathrm{e}^{\alpha a^\dagger}}{\mathrm{e}^{|\alpha|^2/2}}|0\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}}\sum_n \frac{\alpha^n}{\sqrt{n!}}|n\rangle,\ a|\alpha\rangle = \alpha|\alpha\rangle,$$

where the denominator is chosen to normalize $|\alpha\rangle$. Alternatively, by solving the differential equation

$$\langle x|a|\alpha\rangle = \sqrt{\frac{m\omega}{2\hbar}}x\langle x|\alpha\rangle + \mathrm{i}\frac{-\mathrm{i}\hbar}{\sqrt{2m\hbar\omega}}\frac{\partial\langle x|\alpha\rangle}{\partial x} = \alpha\langle x|\alpha\rangle$$

we obtain

$$\langle x|\alpha\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \mathrm{e}^{-\left(\sqrt{\frac{m\omega}{2\hbar}}x-\alpha\right)^2-\frac{1}{2}\alpha(\alpha^*-\alpha)}.$$

The nontrivial normalization here is obtained by considering both $\langle\alpha|\alpha\rangle = 1$ and $\langle 0|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}}$. The coherent states have the most "classical" behavior; we list a few. Express α in polar form $\alpha = |\alpha|\mathrm{e}^{\mathrm{i}\theta}$.

1. Expectation values

$$\langle\alpha|H|\alpha\rangle = \hbar\omega(|\alpha|^2 + \frac{1}{2}),$$

$$\langle\alpha|\hat{x}|\alpha\rangle = \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}\langle\alpha|a+a^\dagger|\alpha\rangle = \frac{1}{2}\sqrt{\frac{2\hbar}{m\omega}}\langle\alpha|\alpha+\alpha^*|\alpha\rangle = \sqrt{\frac{2\hbar}{m\omega}}|\alpha|\cos\theta,$$

$$\langle\alpha|\hat{x}^2|\alpha\rangle = \langle\alpha|\hat{x}|\alpha\rangle^2 + \frac{\hbar}{2m\omega},$$

$$\langle\alpha|\hat{p}|\alpha\rangle = \frac{\sqrt{2m\hbar\omega}}{2\mathrm{i}}\langle\alpha|a-a^\dagger|\alpha\rangle = \sqrt{2m\hbar\omega}|\alpha|\sin\theta,$$

$$\langle\alpha|\hat{p}^2|\alpha\rangle = \langle\alpha|\hat{p}|\alpha\rangle^2 + \frac{m\hbar\omega}{2}.$$

   We see that

$$\langle(\Delta\hat{x})^2\rangle\langle(\Delta\hat{p})^2\rangle = \frac{\hbar^2}{4},$$

   i.e., the coherent state minimizes the uncertainty relation.

2. Time evolution

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}|\alpha\rangle = \mathrm{e}^{-\frac{|\alpha|^2}{2}}\sum_n \frac{\alpha^n}{\sqrt{n!}}\mathrm{e}^{-\mathrm{i}\omega(n+\frac{1}{2})t}|n\rangle = \mathrm{e}^{-\mathrm{i}\omega t/2}|\alpha\mathrm{e}^{-\mathrm{i}\omega t}\rangle.$$

   Therefore,

$$\langle\hat{x}(t)\rangle = \sqrt{\frac{2\hbar}{m\omega}}|\alpha|\cos(\theta-\omega t),\ \langle\hat{p}(t)\rangle = \sqrt{2m\hbar\omega}|\alpha|\sin(\theta-\omega t).$$

   The expectation values of position and momentum are just like the position and momentum of a classical harmonic oscillator.

Problem 3.1.2. Consider, also, the eigen functions of the creation operator $a^\dagger$.

1. Solve in the position basis $\langle x|a^\dagger|\beta\rangle = \beta\langle x|\beta\rangle$.
2. Try to solve in the occupation basis $|n\rangle$. What do you find? Use the eigen function $\langle x|\beta\rangle$ you obtained in the previous step to explain why it is the case.

3.2 Path integral method

Now we switch to the path integral quantization. In this approach one borrows the Lagrangian or action from classical mechanics and then perform the mysterious path integral to obtain the dynamics of the corresponding quantum system. As an infinite dimensional integration, in general the path integral is extremely difficult to carry out. Fortunately, if the action is quadratic, the integrant is Gaussian, and we know how to perform the Gaussian integral exactly. This is the case of harmonic oscillator. However, we will not do the lengthy exact integration here; instead, by analyzing the form of path integral with respect to a general quadratic action, and requiring it to satisfy the composition rule, we obtain (almost) the solution.

The classical path $\bar{x}(t)$ is the stationary point of the action $S[x(t)]$

$$\frac{\delta S}{\delta x(t)}\Big|_{\bar{x}(t)} = 0.$$

Expand the action $S[x(t)]$ around its stationary point

$$S[\bar{x}(t) + \delta x(t)] = S[\bar{x}(t)] + \frac{1}{2}\int \mathrm{d}t_1\, \mathrm{d}t_2\, \frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\Big|_{\bar{x}(t)} \delta x(t_1)\delta x(t_2) + O(\delta x^3).$$

If you feel unconformable with the variational formula, just compare it with a function $f(x_i)$ with multiple input variables indexed by i. Its Taylor expansion is

$$f(x_i + \mathrm{d}x_i) = \sum_n \frac{1}{n!} \sum_{i_1,\ldots,i_n} \frac{\partial^n f}{\partial x_{i_1}\cdots\partial x_{i_n}}\Big|_{x_i} \mathrm{d}x_{i_1}\cdots \mathrm{d}x_{i_n}\,.$$

In the variational case, the time t serves as the continuum index and summation is the integral over t.

For a quadratic action, the expansion stops at second order, thus the path integral becomes

$$\int \mathcal{D}[x(t)] \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S[x(t)]} = F \mathrm{e}^{\frac{\mathrm{i}}{\hbar}S[\bar{x}(t)]},$$

where the prefactor is

$$F = \int \mathcal{D}[\delta x(t)] \exp\left(\frac{\mathrm{i}}{2\hbar}\int \mathrm{d}t_1\, \mathrm{d}t_2\, \frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\Big|_{\bar{x}(t)} \delta x(t_1)\delta x(t_2)\right).$$

Since

1. S is quadratic; its second order variation no longer depends on the path (think about the second derivative of a quadratic polynomial), namely evaluated at any path $x(t)$ we always have the same function $b(t_1, t_2)$ as the second order variation

   $$\frac{\delta^2 S}{\delta x(t_1)\delta x(t_2)}\Big|_{x(t)} = b(t_1, t_2),$$

   where $b(t_1, t_2)$ is determined by the defining parameters (can be time dependant) of S;

2. $\delta x(t) = x(t) - \bar{x}(t)$ has trivial boundary condition

$$\delta x(t_{\text{initial}}) = \delta x(t_{\text{final}}) = 0;$$

we conclude that $F = F(t_{\text{final}}, t_{\text{initial}})$ only depends on the initial and final times but not on the classical path (including the boundary conditions). For simplicity, from now on we assume that the system is time translation invariant, then $F = F(t_{\text{final}} - t_{\text{initial}})$ only depends on the time interval.

Now consider three time points $0, T_1, T_1 + T_2$. The propagator satisfies the composition rule

$$\begin{aligned}\langle x_c, T_1 + T_2 | x_a, 0\rangle &= \int \mathrm{d}x_b \, \langle x_c, T_1 + T_2 | x_b, T_1\rangle \langle x_b, T_1 | x_a, 0\rangle \\ &= \int \mathrm{d}x_b \, \langle x_c, T_2 | x_b, 0\rangle \langle x_b, T_1 | x_a, 0\rangle.\end{aligned}$$

In terms of path integrals

$$F(T_1 + T_2)\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\bar{S}(x_c, x_a, T_1+T_2)} = F(T_1)F(T_2)\int \mathrm{d}x_b \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(\bar{S}(x_c, x_b, T_2) + \bar{S}(x_b, x_a, T_1)\right)},$$

where we use the notation $\bar{S}(x', x, t)$ for $S[\bar{x}(t)]$ with classical path satisfying boundary condition $\bar{x}(0) = x,\ \bar{x}(t) = x'$. To obtain the classical path from $x_a, 0$ to $x_c, T_1 + T_2$, we can consider the path consisting of two segments, classical path from $x_a, 0$ to x_b, T_1 and classical path from x_b, T_1 to $x_c, T_1 + T_2$. The action of the composed path is

$$S(x_c, x_b, x_a, T_2, T_1) = \bar{S}(x_c, x_b, T_2) + \bar{S}(x_b, x_a, T_1).$$

The variation of the above action along the two segments of classical paths is already zero, so we only need to vary it with respect to x_b to obtain the total classical path,

$$\frac{\partial \bar{S}(x_c, x_b, T_2)}{\partial x_b} + \frac{\partial \bar{S}(x_b, x_a, T_1)}{\partial x_b} = 0.$$

The above equation determines $x_b = \bar{x}_b(x_c, x_a)$ as an implicit function of x_a, x_c, and we have

$$\bar{S}(x_c, x_a, T_1 + T_2) = \bar{S}(x_c, \bar{x}_b(x_c, x_a), T_2) + \bar{S}(\bar{x}_b(x_c, x_a), x_a, T_1).$$

Now consider the integral, expanding x_b around $\bar{x}_b(x_c, x_a)$. We further introduce the short-hand notations $\bar{S}_2 = \bar{S}(x_c, x_b, T_2)$, $\bar{S}_1 = \bar{S}(x_b, x_a, T_1)$ and $\bar{S}_{1+2} = \bar{S}(x_c, x_a, T_1 + T_2)$.

$$\begin{aligned}&\int \mathrm{d}x_b \, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left(\bar{S}_2 + \bar{S}_1\right)} \\ &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\bar{S}_{1+2}} \int \mathrm{d}x_b \, \mathrm{e}^{\frac{\mathrm{i}}{2\hbar}\left(\frac{\partial^2 \bar{S}_2}{\partial x_b^2} + \frac{\partial^2 \bar{S}_1}{\partial x_b^2}\right)(x_b - \bar{x}_b)^2} \\ &= \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\bar{S}_{1+2}} \sqrt{\frac{\mathrm{i}2\pi\hbar}{\frac{\partial^2 \bar{S}_2}{\partial x_b^2} + \frac{\partial^2 \bar{S}_1}{\partial x_b^2}}}.\end{aligned}$$

Thus,

$$\frac{F(T_1+T_2)}{F(T_1)F(T_2)} = \sqrt{\frac{\mathrm{i}2\pi\hbar}{\frac{\partial^2 \bar{S}_2}{\partial x_b^2} + \frac{\partial^2 \bar{S}_1}{\partial x_b^2}}}.$$

Examine the following differentials

$$\begin{aligned}
\frac{\partial \bar{S}_{1+2}}{\partial x_c} &= \frac{\partial \bar{S}_2}{\partial x_c} + \frac{\partial \bar{S}_2}{\partial x_b}\Big|_{\bar{x}_b}\frac{\partial \bar{x}_b}{\partial x_c} + \frac{\partial \bar{S}_1}{\partial x_b}\Big|_{\bar{x}_b}\frac{\partial \bar{x}_b}{\partial x_c} = \frac{\partial \bar{S}_2}{\partial x_c},\\
\frac{\partial^2 \bar{S}_{1+2}}{\partial x_c \partial x_a} &= \frac{\partial^2 \bar{S}_2}{\partial x_c \partial x_b}\frac{\partial \bar{x}_b}{\partial x_a},\\
0 &= \frac{\partial}{\partial x_a}\left(\frac{\partial \bar{S}_2}{\partial x_b}\Big|_{\bar{x}_b} + \frac{\partial \bar{S}_1}{\partial x_b}\Big|_{\bar{x}_b}\right) = \left(\frac{\partial^2 \bar{S}_2}{\partial x_b^2} + \frac{\partial^2 \bar{S}_1}{\partial x_b^2}\right)\frac{\partial \bar{x}_b}{\partial x_a} + \frac{\partial^2 \bar{S}_1}{\partial x_b \partial x_a}.
\end{aligned}$$

We obtain

$$\frac{F(T_1+T_2)}{F(T_1)F(T_2)} = \sqrt{-\mathrm{i}2\pi\hbar\frac{\frac{\partial^2 \bar{S}_{1+2}}{\partial x_c \partial x_a}}{\frac{\partial^2 \bar{S}_1}{\partial x_b \partial x_a}\frac{\partial^2 \bar{S}_2}{\partial x_c \partial x_b}}}.$$

Again since the action is quadratic, the second order derivatives only depends on the time interval, so the function $f(T) := F(T)/\sqrt{\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 \bar{S}(x',x,T)}{\partial x' \partial x}}$ satisfies $f(T_1)f(T_2) = f(T_1+T_2)$ and has to be an exponential function, thus

$$F(T) = \sqrt{\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 \bar{S}(x',x,T)}{\partial x' \partial x}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}CT}.$$

$\frac{\partial^2 \bar{S}(x',x,T)}{\partial x' \partial x}$ is known as the *van Vleck determinant* (reducing to just a number in one dimension in our case). At this stage we can only say that C has to be real, otherwise the norm of the propagator either explodes or vanishes as $T \to \infty$, contradicting with unitarity (or conservation of probability). But effectively we can combine CT into the classical action, so the physical meaning of C is merely a constant energy shift and should be able to be dropped safely without affecting physics. Indeed, exact computation shows that $C = 0$. Finally we obtain the *van Vleck-Pauli propagator* for quadratic action

$$\langle x', T|x, 0\rangle = \sqrt{\frac{\mathrm{i}}{2\pi\hbar}\frac{\partial^2 \bar{S}(x',x,T)}{\partial x' \partial x}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\bar{S}(x',x,T)}.$$

Note that when the higher order terms around the classical path does not exactly vanish but negligible, for example when $\hbar \to 0$ or $T \to 0$, the above serves as a good asymptotic approximation, thus it is also referred to as the *semi-classical propagator* or *short-time propagator* in the literature.

We are now ready to compute the propagator of harmonic oscillator, and all we need to do is to find the classical path $\bar{x}(t)$ with respect to the boundary condition $\bar{x}(0) = x,\ \bar{x}(T) = x'$. Due to the periodic nature of the classical solution, we like to assume that $0 < T < \pi/\omega$. Then the desired classical path is

$$\bar{x}(t) = x'\frac{\sin\omega t}{\sin\omega T} + x\frac{\sin(\omega t + \pi - \omega T)}{\sin(\pi - \omega T)}.$$

Thus the action is

$$\begin{aligned} S[\bar{x}(t)] &= \int_0^T \mathrm{d}t\, \frac{1}{2} m \left(\frac{\mathrm{d}\bar{x}}{\mathrm{d}t}\right)^2 - \frac{1}{2} m\omega^2 \bar{x}^2 \\ &= \frac{m\omega}{2\sin\omega T} \left((x^2 + x'^2)\cos\omega T - 2xx' \right), \end{aligned}$$

and

$$\frac{\partial^2 S}{\partial x \partial x'} = -\frac{m\omega}{\sin\omega T}.$$

Therefore, the propagator is

$$\langle x', T|x, 0\rangle = \sqrt{\frac{m\omega}{\mathrm{i}2\pi\hbar\sin\omega T}}\, \mathrm{e}^{\frac{\mathrm{i}m\omega}{2\hbar\sin\omega T}\left((x^2+x'^2)\cos\omega T - 2xx'\right)}.$$

To obtain eigen energies and compare with the results in the last section, we need to find the eigen functions of the propagator

$$\int \mathrm{d}x\, \langle x', T|x, 0\rangle \psi(x) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}ET}\psi(x'),$$

or equivalently, a decomposition of the propagator

$$\langle x', T|x, 0\rangle = \sum_n \phi_n(x')\phi_n^*(x)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_n T},$$

in terms of a complete orthonormal set of functions ϕ_n. By Mehler formula

$$\frac{1}{\sqrt{1-\rho^2}} \exp\left(-\frac{\rho^2(x^2+y^2) - 2\rho xy}{1-\rho^2}\right) = \sum_n \frac{(\rho/2)^n}{n!} H_n(x) H_n(y),$$

it is easy to show $\langle x|n\rangle$ as defined in the last section decompose the propagator. The harmonic oscillator propagator is thus also called the *Mehler kernel*.

Problem 3.2.1. Consider a harmonic oscillator in the gravitational field

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 - mg\hat{x}.$$

Find its energy eigen values and eigen states. Also compute the propagator $\langle x', T|x, 0\rangle$.

Chapter 4

Symmetry and Conserved Quantities

You may have learned in your middle school Newtonian mechanics that when the total external force is zero, the momentum of the system is conserved. Later in undergraduate analytic mechanics course, the statement becomes that when the Hamiltonian/Lagrangian of the system does not depend on coordinates, the corresponding momenta are conserved. In this chapter, we are going to discuss the corresponding formulation in quantum mechanics.

Force is an essential notion in Newtonian mechanics, but becomes deprecated in analytic mechanics. It is represented by the differential of the potential

$$F = -\frac{\partial V}{\partial q}.$$

So independence of coordinates means zero force. In quantum mechanics, we abandoned even more notions in classical mechanics, and introduced quantum exclusive notions such as superposition. We want to answer the two questions:

- The "independence of coordinates" statement still makes sense in quantum mechanics, but only partially. In general, the Hamiltonian is an operator and may act on degrees of freedom beyond coordinates. How to formulate "independence of coordinates" in general operator language?
- The notion of "conserved quantity" has to be generalized because in quantum mechanics any quantity has to be the result of measurements. How to formulate "conserved quantity" in terms of eigenvalue and eigenstate (eigensubspace)?

Before going into details, let's try to answer the questions from only the basic principles of quantum mechanics. First, any measurable quantity should arise as the eigenvalue of some operator. Then, what does it mean for this quantity and this operator to be conserved? In the Hamiltonian approach, this question can

be understood in different pictures. In the Schrodinger picture, the stationary states that only pick up a phase factor under time evolution are the eigenstates of the Hamiltonian H. These states having some quantities conserved means that they should be the eigenstates of the corresponding observable operator O. We conclude that H and O have common eigenstates, thus

$$[H, O] = 0.$$

Alternatively, in the Heisenberg picture, one immediately arrives at

$$0 = \frac{\partial O(t)}{\partial t} = \frac{\mathrm{i}}{\hbar}[H, O(t)].$$

Back to the classical example of coordinates and momenta, in quantum mechanics conserved momentum means

$$[H, \hat{p}] = 0,$$

and again use the "differential" property of commutator,

$$[H, \hat{p}] = \mathrm{i}\hbar \frac{\partial H}{\partial x} = 0,$$

which is indeed consistent with classical mechanics. Now we figured out that

> An observable is conserved when its operator commutes with the Hamiltonian.

But, the relation to coordinates is not satisfactory enough and we will discuss more in the next section.

Another complicity in quantum mechanics is that when there are several conserved observables, say A, B, in the sense

$$[H, A] = 0, \ [H, B] = 0.$$

But A, B are not compatible

$$[A, B] \neq 0.$$

In this case we can not view A, B as conserved quantities respectively, but have to consider them as a whole. The angular momentum in three dimensions is such an example, which will also be discussed in this chapter.

In classical mechanics, many systems can be fully solved by finding all the conserved quantities. It remains true in quantum mechanics. Now what we really need to find is all the operators that commute with the Hamiltonian

$$\mathcal{A} = \{A | [H, A] = 0\}.$$

Such $\mathcal{A}$ is the so called *symmetry* of the system. By studying the algebraic properties of these operators, we could extract most (and sometimes all) information of the system. In many cases, $\mathcal{A}$ is closed related to the notion of *group*. We will finish this chapter by a brief introduction to group theory, while discussing some discrete symmetries.

4.1 Space-time translation, energy and momentum

We have shown that conserved momentum means $[H, \hat{p}] = 0$, then by the canonical commutation relation $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$ one concludes that H is independent of x. However, $[\hat{x}, \hat{p}] = \mathrm{i}\hbar$ is not a natural assumption in the discussion of symmetry and conserved quantities. We try to introduce a more direct and more general point of view.

First, recall our discussion on the evolution and Hamiltonian operator. We are particularly interested in the energy conserved case, and we have the following facts:

- The evolution operator translates time

$$U(t)|\psi(t_0)\rangle = |\psi(t_0 + t)\rangle.$$

- The evolution operator is the exponential of the Hamiltonian

$$U(t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}.$$

- Hamiltonian gives the infinitesimal evolution

$$U(\mathrm{d}t) = 1 - \frac{\mathrm{i}}{\hbar}H\mathrm{d}t + o(\mathrm{d}t)\,,$$

  and is a conserved quantity, the energy.

It worths noting the difference between time and space in non-relativistic quantum mechanics: time is not quantized, only a parameter and not an operator; the states at different times are defined by the evolution operator, and in general do not form an orthonormal basis. On the other hand, space is quantized and we have position operator $\hat{x}$ and orthonormal position states $|x\rangle$ as the eigenstate of $\hat{x}$. Nonetheless, it is a natural and reasonable conjecture that $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}\Delta x}$ translates space. Let's calculate

$$\begin{aligned}
\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}\Delta x}|x\rangle &= \int \mathrm{d}p\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p\Delta x}|p\rangle\langle p|x\rangle \\
&= \int \mathrm{d}p\, \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}p(x+\Delta x)}|p\rangle \\
&= |x + \Delta x\rangle.
\end{aligned}$$

Problem 4.1.1. Verify that $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}\Delta x}$ translates space from the operator point of view by calculating

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}\Delta x}\hat{x}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{p}\Delta x}.$$

Therefore, space translation and momentum has the similar three properties as time translation and energy. We are now ready to conclude the general

picture. Suppose that there is a series of unitary operators $U(r)$ parametrized by a real parameter $r \in \mathbb{R}$, satisfying

$$U(r)U(s) = U(r+s).$$

We can think $U(r)$ as translating the parameter r.

Problem 4.1.2. Verify the properties $U(r)U(s) = U(s)U(r)$, $U(0) = 1$ and $U(-r) = U^\dagger(r)$.

Following a similar derivation as we treat the evolution operator, one can find that

$$A := \mathrm{i}\frac{\partial U(r)}{\partial r}U^\dagger(r) = \mathrm{i}\lim_{\epsilon\to 0}\frac{U(r+\epsilon)-U(r)}{\epsilon}U^\dagger(r) = \mathrm{i}\lim_{\epsilon\to 0}\frac{U(\epsilon)-1}{\epsilon}.$$

is an Hermitian operator that no longer depends on r and

$$U(r) = \mathrm{e}^{-\mathrm{i}Ar}.$$

$U(r)$ is called a one-parameter unitary group (one-dimensional Lie group) and A is the infinitesimal generator of $U(r)$ (one-dimensional Lie algebra). Now the story goes

1. "The Hamiltonian H is independent of parameter r", means the same thing as "H is invariant under translation of r", namely

$$U^\dagger(r)HU(r) = H,\ [H, U(r)] = 0.$$

2. Consequently, the generator A commutes with the Hamiltonian

$$[H, A] = 0,$$

and corresponds to the conserved quantity conjugate to the parameter r.

Problem 4.1.3. Assume that A generates the translation of real parameter r, and in addition, the states defined by

$$|r\rangle := \mathrm{e}^{-\mathrm{i}Ar}|0\rangle,$$

do form an orthonormal basis so that

$$\hat{r} := \int \mathrm{d}r\, |r\rangle r\langle r|,$$

is a valid operator. Compute the commutator

$$[\hat{r}, A].$$

Is this a more natural way to motivate the fundamental commutation relation, comparing to the canonical quantization?

Besides time and energy, position and momentum, another typical example of the above story is angle and angular momentum (in two dimensions). If we try to understand angular momentum in three or more dimensions, we are forced to face the problem of non-compatible conserved quantities, which will be investigated shortly.

One may ask the reversed question, if a system is known to have a conserved quantity, is there always a parameter on which the Hamiltonian does not depend? Unfortunately the answer is no. There are many more different variants of conserved quantities (and symmetries) than Lie groups can cover. We will check a few after the study of angular momentum.

4.2 Rotation and angular momentum

After fixing the center, in two-dimensional space, we only need one parameter to describe rotation; however, in three-dimensional space, we need three parameters, two describing the direction of the axis, and one describing the angle. If the order of two successive rotations are exchanged, the result is the same in two dimensions, but in general different in three dimensions. Such non-commutative nature remains in quantum world, and, as a result, leading to the non-compatibility between the three components of angular momentum.

Let's begin with the quantization of angular momentum in two dimensions. We expect

$$\hat{L}_z = \hat{r} \times \hat{p} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$$

to be the generator of rotation, namely we want to verify

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_z\theta}|x, y\rangle = |x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta\rangle.$$

If we try to apply the operator directly, the following difficulties arise.

1. Since $\hat{x}\hat{p}_y$ does not commute with $\hat{y}\hat{p}_x$, the eigenstates of $\hat{L}$ is totally different from those of $\hat{x}$ or $\hat{p}$.

2. You may then want to turn addition in the exponent to multiplication

   $$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\theta\hat{L}_z} \stackrel{?}{=} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\theta\hat{x}\hat{p}_y}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\theta\hat{y}\hat{p}_x},$$

   and then work with position and momentum basis. However, since the two terms do not commute, there is an correction to the above consisting of infinite terms. (The Baker-Campbell-Hausdorff formula

   $$\mathrm{e}^A\mathrm{e}^B = \mathrm{e}^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]-\frac{1}{12}[B,[A,B]]+\cdots}.$$

   The "$\cdots$" indicates terms involving higher commutators of A and B.)

To bypass these difficulties, a great trick is to study infinitesimal transformations ($\theta \to 0$), in which case the commutator corrections are of second or higher orders of θ.

Up to the first order of $\mathrm{d}\theta$,

$$\begin{aligned}(1-\frac{\mathrm{i}}{\hbar}\hat{L}_z\mathrm{d}\theta)|x,y\rangle &= (1-\frac{\mathrm{i}}{\hbar}\hat{p}_y x\mathrm{d}\theta+\frac{\mathrm{i}}{\hbar}\hat{p}_x y\mathrm{d}\theta)|x,y\rangle \\ &= (1-\frac{\mathrm{i}}{\hbar}\hat{p}_y x\mathrm{d}\theta)(1+\frac{\mathrm{i}}{\hbar}\hat{p}_x y\mathrm{d}\theta)|x,y\rangle.\end{aligned}$$

Since $\hat{p}_x, \hat{p}_y$ generate translations,

$$(1-\frac{\mathrm{i}}{\hbar}\hat{L}\mathrm{d}\theta)|x,y\rangle = |x-y\mathrm{d}\theta, y+x\mathrm{d}\theta\rangle.$$

Thus if we introduce two functions $X(\theta), Y(\theta)$

$$|X(\theta),Y(\theta)\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_z\theta}|x,y\rangle.$$

They satisfy the differential equations

$$\frac{\mathrm{d}X}{\mathrm{d}\theta}=-Y,\ \frac{\mathrm{d}Y}{\mathrm{d}\theta}=X,$$

with initial conditions

$$X(0)=x,\ Y(0)=y.$$

The solution is indeed

$$|X(\theta),Y(\theta)\rangle = |x\cos\theta - y\sin\theta, x\sin\theta+y\cos\theta\rangle.$$

So, $\hat{L}_z$ indeed generates rotation around the z axis. It is completely analogical in three dimensions that $\hat{L}_x=\hat{y}\hat{p}_z-\hat{z}\hat{p}_y$, $\hat{L}_y=\hat{z}\hat{p}_x-\hat{x}\hat{p}_z$ generates rotation around the x and y axes. Before studying a general rotation, we first compute the commutation relations between the three components of angular momentum. Use the compact notation

$$\hat{L}_i=\epsilon_{ijk}\hat{r}_j\hat{p}_k,$$

which assumes Einstein's rule of summation over repeated indices. ϵ_{ijk} is the totally anti-symmetric tensor, $\epsilon_{ijk}=-\epsilon_{jik}=-\epsilon_{ikj}$, and $\epsilon_{xyz}=1$.

$$\begin{aligned}[\hat{L}_i,\hat{L}_j] &= \epsilon_{imn}\epsilon_{jkl}[\hat{r}_m\hat{p}_n,\hat{r}_k\hat{p}_l] \\ &= \epsilon_{imn}\epsilon_{jkl}([\hat{r}_m\hat{p}_n,\hat{r}_k]\hat{p}_l+\hat{r}_k[\hat{r}_m\hat{p}_n,\hat{p}_l]) \\ &= \mathrm{i}\hbar\epsilon_{imn}\epsilon_{jkl}(-\delta_{nk}\hat{r}_m\hat{p}_l+\delta_{ml}\hat{r}_k\hat{p}_n) \\ &= -\mathrm{i}\hbar\epsilon_{imk}\epsilon_{jkl}\hat{r}_m\hat{p}_l+\mathrm{i}\hbar\epsilon_{iln}\epsilon_{jkl}\hat{r}_k\hat{p}_n \\ &= -\mathrm{i}\hbar\epsilon_{imk}\epsilon_{jkn}\hat{r}_m\hat{p}_n+\mathrm{i}\hbar\epsilon_{iln}\epsilon_{jml}\hat{r}_m\hat{p}_n \\ &= \mathrm{i}\hbar\epsilon_{imk}\epsilon_{jnk}\hat{r}_m\hat{p}_n-\mathrm{i}\hbar\epsilon_{inl}\epsilon_{jml}\hat{r}_m\hat{p}_n \\ &= \mathrm{i}\hbar(\epsilon_{imk}\epsilon_{jnk}-\epsilon_{ink}\epsilon_{jmk})\hat{r}_m\hat{p}_n.\end{aligned}$$

Use the identity $\epsilon_{imk}\epsilon_{jnk}=\delta_{ij}\delta_{mn}-\delta_{in}\delta_{jm}$.

$$\begin{aligned}[\hat{L}_i,\hat{L}_j] &= \mathrm{i}\hbar(-\delta_{in}\delta_{jm}+\delta_{im}\delta_{jn})\hat{r}_m\hat{p}_n \\ &= \mathrm{i}\hbar\epsilon_{ijk}\epsilon_{mnk}\hat{r}_m\hat{p}_n \\ &= \mathrm{i}\hbar\epsilon_{ijk}\hat{L}_k.\end{aligned}$$

Indeed they do not commute. We want to emphasize that here we considered only a special case, the *orbital angular momentum*, i.e., the rotation motion in real space. It turns out particles carry *intrinsic angular momentum* that is not related to real space motion and is truly quantum mechanical degree of freedom with no classical counterpart. Although we derive the commutation relations of angular momentum from those of position and momentum operators, for fundamental reasons, we should use the commutation relations as the defining properties of quantum angular momentum; as we will see soon, the commutation relations controls the rotation behavior.

Now, how about a general rotation around an arbitrary axis? In fact, a general rotation can always be decomposed to a sequence of rotations around x, y, z axes. Suppose we want to express a rotation by angle α around the unit vector $\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. What we can do is to

1. First rotate $\boldsymbol{n}$ to the z axis, that is a rotation around z by $-\phi$ followed by a rotation around y by $-\theta$;
2. Second rotate around z by α;
3. Finally rotate z back to $\boldsymbol{n}$, that is a rotation around y by θ followed by a rotation around z by ϕ.

Let's denote the generator of rotation around $\boldsymbol{n}$ by $\hat{L}_{\boldsymbol{n}}$, then

$$\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_{\boldsymbol{n}}\alpha} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_z\phi}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_y\theta}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_z\alpha}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{L}_y\theta}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{L}_z\phi}.$$

Again, we can determine $\hat{L}_{\boldsymbol{n}}$ by considering infinitesimal α, which leads to

$$\hat{L}_{\boldsymbol{n}} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_z\phi}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{L}_y\theta}\hat{L}_z\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{L}_y\theta}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}\hat{L}_z\phi}.$$

Remember that we have explored how to solve the operator of the form

$$\mathrm{e}^{At}B\mathrm{e}^{-At} = \mathrm{e}^{[A,-]t}B$$

when we study quantum evolutions; it resembles an operator in the Heisenberg picture. Thus

$$\hat{L}_{\boldsymbol{n}} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[L_z,-]\phi}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[L_y,-]\theta}\hat{L}_z.$$

It is not hard to see the action of $[L_y, -]$ just swaps L_z and L_x, so we have

$$\begin{aligned}\hat{L}_{\boldsymbol{n}} &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[L_z,-]\phi}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[L_y,-]\theta}\hat{L}_z \\ &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}[L_z,-]\phi}(\hat{L}_z\cos\theta + \hat{L}_x\sin\theta) \\ &= \hat{L}_z\cos\theta + \hat{L}_x\sin\theta\cos\phi + \hat{L}_y\sin\theta\sin\phi.\end{aligned}$$

It agrees with the component of the angular momentum along $\boldsymbol{n}$, which in classical mechanics is $\boldsymbol{L}\cdot\boldsymbol{n} = L_x\sin\theta\cos\phi + L_y\sin\theta\sin\phi + L_z\cos\theta$. Thus we can write $\hat{L}_{\boldsymbol{n}} = \hat{\boldsymbol{L}}\cdot\boldsymbol{n}$. Note that in the above we did not use the orbital angular momentum expression $\hat{L}_i = \epsilon_{ijk}\hat{r}_j\hat{p}_k$; we used only the fundamental

commutation relation of angular momentum and thus the above discussion also applies to intrinsic angular momentum. Conversely, assuming the rotation rules, one can derive the fundamental commutation relation of the generators; this relation in general is known as the Lie group – Lie algebra correspondence, and in the rotation case the $SO(3)$ Lie group and $\mathfrak{su}(2)$ Lie algebra.

Problem 4.2.1. The rotation in three-dimensional space can be described by 3×3 orthogonal matrices with determinant 1, hence the name $SO(3)$ (special orthogonal group of dimension 3).

1. Write down the 3×3 matrices $R_x(\alpha),\ R_y(\alpha),\ R_z(\alpha)$ for rotations around x, y, z axes by angle α.

2. Assuming that α is small, find the generators G_i, as 3×3 matrices, of infinitesimal rotations

$$R_i(\alpha) = 1 + \alpha G_i + O(\alpha^2), \quad i = x, y, z.$$

3. Calculate the commutators between G_i and compare them to those of the angular momentum operators $\hat{L}_i$.

The total angular momentum consists of two parts $J_i = \hat{L}_i + S_i$, where $\hat{L}_i = \epsilon_{ijk}\hat{r}_j\hat{p}_k$ is the orbital angular momentum and S_i is the intrinsic angular momentum or *spin*. In non-relativistic quantum mechanics, the origin of intrinsic angular momentum can not be explained; it is observed in experiments and put into theory by hand. Like the orbital one, the total and intrinsic angular momentum both satisfy the commutation relation

$$[J_i, J_j] = \mathrm{i}\hbar\epsilon_{ijk}J_k,\ [S_i, S_j] = \mathrm{i}\hbar\epsilon_{ijk}S_k.$$

$\hat{L}_i$ acts on the position space, whose eigenstates can be found by solving the corresponding differential equations (we will discuss it later). But for the spin S_i, we don't even know, a priori, which Hilbert space it is acting on. What we know is only that they are angular momentum, thus should generate rotation, or equivalently, satisfy the fundamental commutation relation. So our question here is to identify the proper Hilbert space V such that J_i or S_i are operators acting on V that satisfy the commutation relation. In more abstract language, the question is to find the representation of Lie algebra or Lie group describing the desired symmetry (rotation here). More precisely, we want to find the smallest Hilbert space V to realize the commutation relation, in the sense there is no subspace $M \subsetneqq V$ such that $J_iM \subset M$ except the zero space. In this process, you can feel how powerful the algebraic relation is.

First, since J_x, J_y and J_z do not commute, there is no simultaneous eigenstate of all three components. We can, at most, choose the eigenstates of one of the three, which is by convention usually J_z, and then express the other two, J_x, J_y, in terms of the eigenstates of J_z. Moreover, if there is some operator which is a combination of J_x, J_y and commutes with J_z, then we may work in

the common eigensubspace of this operator and J_z, which could greatly simplify the problem.

$[J_z, -]$ swaps J_x and J_y so an operator linear in J_x and J_y won't commute with J_z. Let's try the quadratic terms $J_x^2, J_y^2, J_xJ_y, J_yJ_x$.

$$\begin{aligned}
[J_z, J_x^2] &= [J_z, J_x]J_x + J_x[J_z, J_x] = \mathrm{i}\hbar(J_yJ_x + J_xJ_y),\\
[J_z, J_y^2] &= [J_z, J_y]J_y + J_y[J_z, J_y] = -\mathrm{i}\hbar(J_xJ_y + J_yJ_x),\\
[J_z, J_xJ_y] &= [J_z, J_x]J_y + J_x[J_z, J_y] = \mathrm{i}\hbar(J_y^2 - J_x^2),\\
[J_z, J_yJ_x] &= [J_z, J_y]J_x + J_y[J_z, J_x] = \mathrm{i}\hbar(J_y^2 - J_x^2).
\end{aligned}$$

$J_xJ_y - J_yJ_x$ does not help because it is simply proportional to J_z. $J_x^2 + J_y^2$ is the operator we seek for, but it is not good enough. Since we want a Hilbert (sub)space on which all of J_x, J_y, J_z act on, we take the sum of all three components squared

$$J^2 := J_x^2 + J_y^2 + J_z^2.$$

It is not hard to see J^2 commutes with all three components J_x, J_y, J_z. The action of J_x, J_y or J_z does not change the eigenvalue of J^2, namely, they acts within an eigensubspace. So, we like to take an eigensubspace of J^2, and then decompose the eigensubspace according to the eigenvalues of J_z. Now we are facing the eigenvalue problem

$$J^2 - J_z^2 = J_x^2 + J_y^2.$$

You see that it is quite similar to the harmonic oscillator problem. We attempt to define

$$J_+ = J_x + \mathrm{i}J_y,\ J_- = J_x - \mathrm{i}J_y.$$

Their commutation relations with J_z are

$$\begin{aligned}
[J_z, J_+] &= \hbar J_+\\
[J_z, J_-] &= -\hbar J_-.
\end{aligned}$$

Thus, given an eigenstate $|\psi\rangle$ of J_z, $J_z|\psi\rangle = m\hbar|\psi\rangle$,

$$J_zJ_+|\psi\rangle = (J_+J_z + \hbar J_+)|\psi\rangle = (m+1)\hbar J_+|\psi\rangle.$$

If $J_+|\psi\rangle$ is not zero, its eigenvalue (angular momentum along z) is increased by one unit of $\hbar$. (The important constant $\hbar$ now clarifies its physical meaning as the quantum of angular momentum.) Similarly, J_- decreases angular momentum along z by $\hbar$.

Problem 4.2.2. In a more general setting, verify the following statement: given an operator A, the eigen operator of $[A, -]$ with eigenvalue λ translates the eigenvalue of A by λ. Find the eigen operator of $[J_z, -]$ in the operator space spanned by J_x J_y and J_z.

Like in the harmonic oscillator problem, the non-negativity of $J_x^2 + J_y^2 = J^2 - J_z^2$ gives a bound that constraints the possible range of J_z eigenvalues. Clearly J_z should have both an upper and lower bound since $J^2 - m^2\hbar^2 \geq 0$.

For the largest eigenvalue $m_{\max}\hbar$ and eigenstate $|\psi_{\max}\rangle$, we must have

$$J_+|\psi_{\max}\rangle = (J_x + \mathrm{i}J_y)|\psi_{\max}\rangle = 0.$$

Using the above relation we can compute

$$(J_x^2 + J_y^2)|\psi_{\max}\rangle = (-\mathrm{i}J_xJ_y + \mathrm{i}J_yJ_x)|\psi_{\max}\rangle = \hbar J_z|\psi_{\max}\rangle = m_{\max}\hbar^2|\psi_{\max}\rangle,$$

and

$$J^2|\psi_{\max}\rangle = (m_{\max}^2 + m_{\max})\hbar^2|\psi_{\max}\rangle.$$

For the smallest eigenvalue $m_{\min}\hbar$ and eigenstate $|\psi_{\min}\rangle$ we have

$$J_-|\psi_{\min}\rangle = 0,\ J^2|\psi_{\min}\rangle = (m_{\min}^2 - m_{\min})\hbar^2|\psi_{\min}\rangle.$$

We are working within the eigensubspace of J^2, thus

$$m_{\max}^2 + m_{\max} = m_{\min}^2 - m_{\min},$$

which leads to

$$m_{\min} = -m_{\max}.$$

Conventionally, we denote by $j = m_{\max} = -m_{\min}$ the largest magnitude of angular momentum. Then the eigenvalue of J^2 is $j(j+1)\hbar^2$ (not $j^2\hbar^2$). $2j = m_{\max} - m_{\min}$ has to be an integer, so we conclude the possible values of j are the half integers $0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$

Since we want a minimal space that the angular momentum operators act on, let's pick one eigenstate of J_z with eigenvalue $j\hbar$, and apply J_- to generate other eigenstates. Let $|j,j\rangle$ be a normalized state with $J^2|j,j\rangle = j(j+1)\hbar^2|j,j\rangle$, $J_z|j,j\rangle = j\hbar|j,j\rangle$. Define $|j,m\rangle = C_m J_-^{l-m}|j,j\rangle$ where C_m is a normalization factor. We determine the normalization inductively

$$\begin{aligned}\langle j,m|J_-^\dagger J_-|j,m\rangle &= \langle j,m|J_+J_-|j,m\rangle \\ &= \langle j,m|(J_x^2 + J_y^2 + \hbar J_z)|j,m\rangle \\ &= (j(j+1) - m^2 + m)\hbar^2 = (j+m)(j-m+1)\hbar^2.\end{aligned}$$

Therefore, we should define inductively

$$|j,m-1\rangle := \frac{1}{\sqrt{(j+m)(j-m+1)}\hbar}J_-|j,m\rangle.$$

We also see that $\langle j,-j|J_-^\dagger J_-|j,-j\rangle = 0$ which is consistent. Now we express J_+ in terms of these eigenstates $|j,m\rangle$

$$\begin{aligned}J_+|j,m\rangle &= J_+\frac{1}{\sqrt{(j+m+1)(j-m)}\hbar}J_-|j,m+1\rangle \\ &= \frac{1}{\sqrt{(j+m+1)(j-m)}\hbar}(J_x^2 + J_y^2 + \hbar J_z)|j,m+1\rangle \\ &= \sqrt{(j-m)(j+m+1)}\hbar|j,m+1\rangle.\end{aligned}$$

Now we have established a Hilbert space V_j spanned by $|j,m\rangle$, where j is an half integer and $m = -j, -j+1, \ldots, j-1, j$. The angular momentum operators act on this space by

$$\begin{aligned} J_z|j,m\rangle &= m\hbar|j,m\rangle, \\ J_\pm|j,m\rangle &= \sqrt{(j\mp m)(j\pm m+1)}\hbar|j,m\pm 1\rangle, \\ J_x = \frac{1}{2}(J_+ + J_-),\ J_y &= \frac{\mathrm{i}}{2}(J_- - J_+). \end{aligned}$$

Problem 4.2.3. Use the explicit operator actions above to verify that they indeed satisfy the angular momentum commutation relation.

This space is indeed minimal: assume that M is a subspace of V_j invariant under actions of J_i. Then by $J_z M = M$ there must an eigenstate of J_z in M. Then applying J_+ and J_- to this eigenstate generates all the eigenstates of J_z, therefore, $M = V_j$. In mathematical term, V_j is an irreducible representation of the Lie algebra $\mathfrak{su}(2)$ (angular momentum operators).

The above is the quantum description of angular momentum. Unlike in classical mechanics where angular momentum is just a three-component vector, in quantum mechanics, angular momentum is described by a Hilbert space V_j labeled by an half integer j, together with the rules how J_i act on this space V_j. This representation V_j is the quantum version of conserved quantity of angular momentum. It is no longer simply some numbers; it is numbers and states (a vector space) with additional structures.

Now let's go through some examples:

Spin 0 Only one basis state $|0,0\rangle$ with $J^2|0,0\rangle = J_z|0,0\rangle = 0$.

Spin $\frac{1}{2}$ Two basis states $|\frac{1}{2}, \pm\frac{1}{2}\rangle$. Angular momentum operators are proportional to the Pauli operators $J_i = \frac{1}{2}\hbar\sigma_i$.

Orbital angular momentum In polar coordinates,

$$\begin{aligned} \hat{L}^2 &= \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \\ &= \hbar^2\left(-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \\ \hat{L}_z &= -\mathrm{i}\hbar\frac{\partial}{\partial\phi}. \end{aligned}$$

And the eigen functions $Y_l^m(\theta,\phi)$ of

$$\hat{L}^2 Y_l^m = l(l+1)\hbar^2 Y_l^m,\ \hat{L}_z Y_l^m = m\hbar Y_l^m,$$

turns out to be the spherical harmonic functions, but only for integer l. Half integer angular momenta are truly quantum. The spherical harmonic functions form a convenient basis if the system has spherical symmetry (i.e. only depends on r, no dependence on direction θ, ϕ).

4.3 Group and representation

Now let's discuss *symmetry* and conserved quantity in a more general setting. Similar to the translation and rotation, we may apply any operation to our system, and if the system remains invariant after the operation, we may say that the system has some symmetry.

We first discuss the abstract properties of these *operations*, without referring to any specific system. Denote the possible operations by $g, h, \ldots$

1. Two successive operations g followed by h, is still an operation, which is denoted by $h \circ g$, or more compactly just hg.

2. "No operation" constitutes a special operation, denoted by 1. Clearly

$$1 \circ g = g \circ 1 = g,$$

   for any operation g.

3. Three successive operations g followed by h followed by l, should be the same as applying the operations two by two, namely

$$l \circ (h \circ g) = (l \circ h) \circ g.$$

4. As the system remains invariant, for any operation g, there should an operation g^{-1} which reverse the system back to its original state, namely

$$g^{-1} \circ g = 1.$$

   And also (you can easily prove it or simply use it as an axiom)

$$g \circ g^{-1} = 1.$$

Collect all these operations $g, h, \ldots$ to form a set, we arrives at the definition of a **group**: a set G equipped with an associative binary operation (called multiplication) $\circ : G \times G \to G$ that has identity element 1 and inverse.

The abstract mathematical theory of group is already rich itself, but here we care more about its application in quantum mechanics. In particular, instead of the abstract operations or group elements, we want to represent them in terms of concrete operators. This idea leads to the notion of group representation.

Denote by $GL(V)$ the set of *invertible operators* on a vector space $V \to V$. Define the multiplication to be just the operator composition, and it is easy to verify that $GL(V)$ is a group.

A group homomorphism is a map $f : G \to H$ between groups G and H that preserves multiplication $f(hg) = f(h)f(g)$. The notion is useful in the sense that if we know the properties of G, they can be carried over via f to the group H. And here we want to take $H = GL(V)$ to be a very concrete group: a representation of group G is a pair (V, ρ) where V is a vector space and $\rho : G \to GL(V)$ is a group homomorphism. In particular, if a basis $|i\rangle$ of V

is chosen, the image $\rho(g)$ of group element g under ρ can be represented more concretely by a matrix $\langle i|\rho(g)|j\rangle$. Thus it is also often seen in the literature that a representation means a collection of matrices U_g labeled by group elements, such that $U_h U_g = U_{hg}$. This style of language, though concrete, has some weak points: 1) the change of basis has to be accounted by saying two representations to be equivalent if they differ by a similarity transformation $U'_g = PU_gP^{-1}$; 2) hiding the underlying Hilbert space V sometimes leads to overlook at the physical picture.

The group representation (V, ρ) is exactly the mathematical description for conserved quantity, corresponding to the mathematical description, group, for symmetry. To see this, we may look at a 1-dimensional representation. In this case, the basis state $|b\rangle$ of V is just an eigenstate of all group actions $\rho(g)$, since for any g, $\rho(g)|b\rangle$ has to be $|b\rangle$ times some non-zero number b_g, which is then related to some conserved observable. As an example, consider the translation symmetry. As an abstract group, we may say the translation is just the real numbers x with group multiplication given by addition $x_1 + x_2$. A representation on the Hilbert space spanned by the 1-dimensional position basis is then $\rho(x) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}x}$. We see that each momentum state spans a 1-dimensional representation of the translation symmetry

$$\rho(x)|p\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}|p\rangle.$$

To understand the nature of conservation better, the notion of irreducible representation introduced in the last section plays an important role. We are going to show that if the system has symmetry, it is impossible for an irreducible representation to evolve into a different irreducible representation. Intuitively, an irreducible representation is a "smallest" one. Given a representation (V, ρ), suppose that we can find a subspace $W \subset V$ such that $\rho(g)W \subset W$, then we obtain a sub-representation $(W, \rho|_W)$ where $\rho|_W(g)$ is just the restriction $\rho(g)|_W$ of $\rho(g)$ on the subspace W. Clearly $W = 0$ or $W = V$ is always a sub-representation. A representation (V, ρ) is called irreducible if, besides 0 and V itself, there is no other subspace W satisfying $\rho(g)W \subset W$ for all g. Another useful notion is the *intertwiner*: an linear map $f : W \to V$ between two representations (W, β) and (V, ρ) is called an intertwiner if it commutes with group actions

$$f\beta(g) = \rho(g)f, \quad \forall g.$$

We have Schur's lemma: an intertwiner between two irreducible representations is either zero or an invertible map. This lemma follows directly from the fact that $\ker f$ and fW are sub-representations of W and V respectively. As W, V are assumed irreducible, we can only have $\ker f = W, fW = 0$ (zero map) or $\ker f = 0, fW = V$ (invertible map).

The intertwiner arises naturally in physics. A system with Hilbert space V and Hamiltonian H has symmetry G means:

1. There is a group representation $\rho : G \to GL(V)$ that realize the group actions as operators $\rho(g)$ on the physical Hilbert space V;

2. The Hamiltonian commutes with all group actions

$$[H, \rho(g)] = 0, \quad \forall g \in G.$$

In other words, H, as well as the time evolution $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}$, are intertwiners.

The total Hilbert space V is in general reducible; however, we can always decompose V to subspaces $W \subset V$ that are irreducible. Now, according to Schur's lemma and the continuity of evolution, a state $|\psi\rangle \in W$ in an irreducible representation, after time evolution, has to remain in the same irreducible representation, $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}Ht}|\psi\rangle \in W$. This phenomenon is also known as the *(super-)selection rule*. We see the irreducible representation, as a whole, corresponds to the conserved quantity of the symmetry.

Next we examine several examples of important symmetries beyond translation and rotation.

Parity and mirror symmetry The parity symmetry is given by

$$P|\boldsymbol{r}\rangle = |-\boldsymbol{r}\rangle.$$

It reverse all the position coordinates. The mirror symmetry, on the other hand, only reflects one direction, for example the y-z plane as the mirror plane,

$$M_x|x, y, z\rangle = |-x, y, z\rangle.$$

Clearly $P^2 = 1 = M_x^2$. The parity and mirror symmetries both have $\mathbb{Z}_2$ as the abstract group, but realized differently in the physical Hilbert space (different representations), they are different symmetries. Anyways, in 1-dimensional space they are the same. We can derive the parity action on momentum states, as well as on operators

$$P|p\rangle = \int \mathrm{d}x \, \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}|-x\rangle = \int \mathrm{d}x \, \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}|x\rangle = |-p\rangle,$$
$$P\hat{x}P = -\hat{x}, \quad P\hat{p}P = -\hat{p}.$$

So, the orbital angular momentum $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$ under parity is

$$P\hat{L}_i P = \hat{L}_i.$$

We expect the total angular momentum, as well as the spin, to satisfy the same relation

$$PJ_iP = J_i, \quad PS_iP = S_i.$$

The above is used as the fundamental assumption to determine how parity should act on the internal degrees of freedom of particles, usually the spin degrees of freedom.

The application of parity symmetry, follows from the general discussion, is that we can divide the states into two sectors, even and odd, according to their

eigenvalues under parity action $P|\psi\rangle = \pm|\psi\rangle$. Even and odd states will never touch the other under parity-symmetric evolutions.

Discrete/Lattice translation symmetry

In many-body physics, a typical problem is that atoms reside in a lattice and provide a periodic background potential in which the electron moves. When the potential $V(x)$ is periodic $V(x) = V(x+a)$, the discrete translation operator

$$T_a|x\rangle = |x+a\rangle, \quad T_a = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}a},$$

generates a discrete translation symmetry $\{T_a^n\}$. The abstract group here is the same as the integers. The irreducible representations are still given by momentum states. But note that $|p\rangle$ and $|p + 2\pi\hbar/a\rangle$ give rise to the same eigenvalue of the discrete translation operator T_a; therefore, effectively, discrete position truncate momentum down to a finite range with a periodic boundary condition.

We may further assume that our system is finite in space and impose the periodic boundary condition $|x + L\rangle = |x\rangle$ (or think that the system is put on a ring with perimeter L), and the discrete lattice has N sites $L = Na$. Then we have $T_a^N = 1$; the group becomes $\mathbb{Z}_N$. Moreover, the momentum also gets quantized, since

$$T_a^N = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}aN} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{p}L} = 1,$$

thus

$$\frac{pL}{\hbar} = 2\pi k, \quad k \in \mathbb{Z}.$$

The momentum eigenvalues can only be multiples of $\frac{2\pi\hbar}{L}$.

Time-reversal symmetry The so-called time-reversal symmetry is beyond our previous discussion, since linear operators do not suffice for representing time-reversal symmetry. We need some additional treatment. The name is a bit misleading: in fact we don't really want to reversal the time; instead, we want to study what happens if we reverse the direction of motion. That is, we want an operator T to act as

$$T|x\rangle = |x\rangle, \quad T|p\rangle = |-p\rangle,$$

reversing momentum while keeping position unchanged. However, unlike in classical mechanics, $|x\rangle$ and $|p\rangle$ are not independent in quantum mechanics. If T is an linear operator, the above formulas are impossible. We have to generalize the notion of operators: An **antilinear** operator $A : V \to W$ between Hilbert spaces V, W is a map satisfying

$$A(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^* A|\alpha\rangle + c_2^* A|\beta\rangle.$$

If T is antilinear and $T|x\rangle = |x\rangle$, we can check

$$\begin{aligned} T|p\rangle &= \int \mathrm{d}x \, \frac{1}{\sqrt{2\pi\hbar}} T \mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}|x\rangle \\ &= \int \mathrm{d}x \, \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px} T|x\rangle \\ &= \int \mathrm{d}x \, \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}px}|x\rangle \\ &= |-p\rangle. \end{aligned}$$

So an antilinear operator gives the desired property of only reversing the direction of motion.

An antilinear operator is not easy to deal with. Note that if A and B are both antilinear, then AB is linear. So a common trick is to choose a fixed antilinear operator, usually called *complex conjugation* operator, and usually denoted by K. But again the name is a bit misleading (as is very common in the field of time-reversal symmetry). It makes no sense to say whether a state vector is real, complex, or imaginary. What this K operator really does is that it acts on a chosen orthogonal basis $|b\rangle$ trivially

$$K|b\rangle = |b\rangle,$$

and then extends to the whole space by antilinearity. So strictly speaking, such K depends on basis choice, however, unfortunately the basis choice is almost never made explicit in the literature. Anyways, it can be checked that $K^2 = 1$. For an arbitrary antilinear operator A, AK is linear, $A = (AK)K$. Therefore, one can express any antilinear operator as

$$A = LK,$$

where L is linear and K is a complex conjugate operator (for a chosen basis, as we explained). In particular if L in the above is unitary, A is called anti-unitary, or equivalently, antilinear operator A is called anti-unitary if $\langle A\alpha|A\beta\rangle = \langle\alpha|\beta\rangle^*$.

To conclude, time-reversal symmetry needs to be represented by an anti-unitary operator T. Acting on position and momentum operators,

$$T\hat{x}T^{-1} = \hat{x}, \quad T\hat{p}T^{-1} = -\hat{p}.$$

Thus, for the angular momentum we have

$$TJ_iT^{-1} = -J_i.$$

Problem 4.3.1. Determine the time-reversal operator T acting on a spin 1/2 particle. Let $|0\rangle, |1\rangle$ be the eigen basis of σ_z and choose the complex conjugation operators K to act trivially on $|0\rangle, |1\rangle$. Express T as $T = UK$ where U is a unitary operator. Use the assumptions

$$T\sigma_iT^{-1} = -\sigma_i,$$

namely

$$UK\sigma_i KU^\dagger = -\sigma_i.$$

You should find a unique solution, up a phase factor. Calculate T^2. What is the abstract group for time-reversal acting on spin 1/2?

Hint: First compute $K\sigma_i K$ which is a linear operator. $1, \sigma_i, i = x, y, z$ form a basis of operators, so you can always write $U = a_0 + \sum_i a_i\sigma_i$ for complex numbers a_i.

Chapter 5

Many-body Theory

In this chapter we discuss some basic ingredients of many-body theory.

5.1 Composite system and tensor product

Let's start by considering how to construct a many-body system. Clearly as the name indicates, a many-body system includes many one-body subsystems. It should be possible to construct firstly a two-body system, by composing two one-body systems; next we can view the two-body system as a larger one-body system, and compose it with another one-body system, to obtain a three-body system; so on and so forth we can have an as-many-as-possible-body system.

Thus, let's investigate, based on the general quantum mechanics principles, what it means by a composite system consisting of two subsystems, i.e., a two-body system.

Recall that we need to identify a physical system by measurements, in other words, identify the Hilbert space by the spectrum of possible observables. When we say a system can be divided into two subsystems, from a measurement perspective, we in fact mean

1. Each subsystem can be measured independently. For simplicity, let's say we have two operators A and B. A measures the states of subsystem 1, according to which we identify the Hilbert space V_1 of subsystem 1 by the eigenstates of A, $A|a\rangle = a|a\rangle$; V_1 is spanned by $|a\rangle$. Similarly, B measures the states of subsystem 2, and we identify V_2 spanned by $|b\rangle$, $B|b\rangle = b|b\rangle$.

2. The states of the total system, composed by subsystems 1 and 2, should be fully determined when we know the states for both subsystems. Namely, the total Hilbert space V is spanned by $|a, b\rangle$ where $A|a, b\rangle = a|a, b\rangle$, and $B|a, b\rangle = b|a, b\rangle$. In particular, we see that $|a, b\rangle$ are common eigenstates of A and B. The operators acting on different subsystems are automatically compatible.

3. We also need to consider superpositions. V_1, V_2 and V are both Hilbert spaces; if we have a general state, not an eigen basis, in V_1 or V_2, what should be the corresponding state in the total space V? It is natural to require that V inherits the linearity of V_1 and V_2. From now on we drop the assumption that $|a\rangle$ and $|b\rangle$ are eigenstates of some operators, and use them for generic states in subsystems 1 and 2 respectively. For subsystem states

$$c_1|a_1\rangle + c_2|a_2\rangle \in V_1, \quad |b\rangle \in V_2,$$

the total state is

$$c_1|a_1, b\rangle + c_2|a_2, b\rangle.$$

Similarly, for subsystem states

$$|a\rangle \in V_1, \quad c_1|b_1\rangle + c_2|b_2\rangle \in V_2,$$

the total state is

$$c_1|a, b_1\rangle + c_2|a, b_2\rangle.$$

You can see that the naive notation $|a, b\rangle$ is not convenient when dealing with superpositions (linear combinations), and thus also change of basis if we want to measure subsystems using some other observables. It is instructive to seek for a basis independent description of the total Hilbert space. We begin by putting the states of subsystems together, i.e., that Cartesian product $V_1 \times V_2 = \{(|a\rangle, |b\rangle)||a\rangle \in V_1, |b\rangle \in V_2\}$. $V_1 \times V_2$ is merely a set; next we make $V_1 \times V_2$ a vector space by taking all formal linear combinations $\sum c_{a,b}(|a\rangle, |b\rangle)$, denoted by $F(V_1 \times V_2)$, the free vector space over the set $V_1 \times V_2$. Clearly $F(V_1 \times V_2)$ is too large; any $(|a\rangle, |b\rangle)$ is a basis vector. We then introduce an equivalence relation $\sim$:

$$(c_1|a_1\rangle + c_2|a_2\rangle, |b\rangle) \sim c_1(|a_1\rangle, |b\rangle) + c_2(|a_2\rangle, |b\rangle),$$
$$(|a\rangle, c_1|b_1\rangle + c_2|b_2\rangle) \sim c_1(|a\rangle, |b_1\rangle) + c_2(|a\rangle, |b_2\rangle).$$

And define the total Hilbert space to be the quotient set

$$V_1 \otimes V_2 := F(V_1 \times V_2)/\sim,$$

called the tensor product of V_1 and V_2. Also, we use the notation $|a\rangle \otimes |b\rangle$ for a state vector in $V_1 \otimes V_2$, representing the equivalence class containing $(|a\rangle, |b\rangle)$. Then we have equations

$$(c_1|a_1\rangle + c_2|a_2\rangle) \otimes |b\rangle = c_1|a_1\rangle \otimes |b\rangle + c_2|a_2\rangle \otimes |b\rangle,$$
$$|a\rangle \otimes (c_1|b_1\rangle + c_2|b_2\rangle) = c_1|a\rangle \otimes |b_1\rangle + c_2|a\rangle \otimes |b_2\rangle.$$

We also have the tensor product of operators $A \otimes B$, which is defined by acting on the states component-wise, $(A \otimes B)(|a\rangle \otimes |b\rangle) = (A|a\rangle) \otimes (B|b\rangle)$. It follows directly that the composition of operators is also component-wise

$$(A \otimes B)(U \otimes W) = (AU \otimes BW).$$

An operator A acting on V_1 becomes an operator $A \otimes 1$ acting on the tensor product $V_1 \otimes V_2$. Similarly for an operator B acting on V_2. It follows directly from the definition that

$$(A \otimes 1)(1 \otimes B) = A \otimes B = (1 \otimes B)(A \otimes 1).$$

So strictly speaking, it is $A \otimes 1$ that commutes with $1 \otimes B$.

Problem 5.1.1. The construction of total Hilbert space (tensor product) using a chosen basis is more convenient in practice, that is, fix the bases $|a\rangle$ of V_1 and $|b\rangle$ of V_2, let $V_1 \otimes V_2$ be a vector space with basis $|a\rangle \otimes |b\rangle$, and extend from basis to generic state by linearity.

1. Prove that such construction is indeed basis independent, that is, even if one chooses different bases of V_1 and V_2, the constructed $V_1 \otimes V_2$ differs by only a change of basis.

2. Denote the operators acting on V by $\mathrm{Hom}(V, V)$. Prove that

$$\mathrm{Hom}(V_1 \otimes V_2, V_1 \otimes V_2) = \mathrm{Hom}(V_1, V_1) \otimes \mathrm{Hom}(V_2, V_2).$$

   Hint: Pick a basis $|a\rangle$ of V, then a basis of the operator space is $|a\rangle\langle a'|$.

3. Write down the matrix elements of $A \otimes B$ in terms of matrix elements of A and B.

Therefore, to compose two systems into one, we just take the tensor product. Repeat the procedure we can compose any numbers of systems into one

$$(\cdots((V_1 \otimes V_2) \otimes V_3) \otimes \cdots \otimes V_n).$$

One thing to note is that the associativity of the tensor product

$$(V_1 \otimes V_2) \otimes V_3 \simeq V_1 \otimes (V_2 \otimes V_3)$$

is by no means a simple equality, but requires an invertible linear map to identify

$$(|a\rangle \otimes |b\rangle) \otimes |c\rangle \leftrightarrow |a\rangle \otimes (|b\rangle \otimes |c\rangle).$$

You can see the vectors on either side have quite different meanings in our construction of tensor product. There is in fact no alternative construction which can make the tricky difference vanish. Nevertheless, the above identification is so natural that in practice it is always assumed implicitly and then the brackets are dropped. However, noticing a trivial structure is the first step towards finding non-trivial structures. Indeed it is possible to identify $(V_1 \otimes V_2) \otimes V_3$ and $V_1 \otimes (V_2 \otimes V_3)$ using some different linear maps other than the most natural one, and such consideration leads you to the realm of tensor category theory.

It becomes a technical difficulty how to express the states and operators when there are too many subsystems (a long tensor product sequence). People invented various shorthand notations in the literature:

1. The tensor product notation is preferred in mathematics literature. It is clear but a bit long. An advantage is that you can use the tensor product symbol to express some general formula (if there exists one), such as

$$\otimes_{i=1}^{n}(|a_i\rangle + c_i|b_i\rangle) = (|a_1\rangle + c_1|b_1\rangle) \otimes \cdots \otimes (|a_n\rangle + c_n|b_n\rangle).$$

   Also when you do not want to use the quantum mechanical bracket notations, but want to use a single letter a to represent a vector, the tensor product notation seems your best choice.

2. Drop the tensor product and simply put kets and bras side by side:

$$|a\rangle|b\rangle := |a\rangle \otimes |b\rangle, \quad \langle a|\langle b| := \langle a| \otimes \langle b|.$$

   For operators, similarly

$$XIZZY := X \otimes 1 \otimes Z \otimes Z \otimes Y,$$

   which is often seen in quantum information literatures. Note that you can not omit identity operators in this notation.

3. Further drop the brackets in the middle:

$$|ab\rangle := |a\rangle \otimes |b\rangle, \quad \langle ab| := \langle a| \otimes \langle b|.$$

   Or use some other separators like $|a, b\rangle$, especially when a, b are some longer labels. This style of notations make the state vector short, but are not convenient to deal with operators.

4. For operators, the indexed notation is more often used, especially for many-body cases. Just put an index around the operator to specify on which subsystem it is acting on.

$$A^{(1)} = A \otimes 1 \otimes 1 \otimes \cdots, \quad B^{(2)} := 1 \otimes B \otimes 1 \otimes \cdots.$$

As an application, let's discuss the addition of conserved quantities of subsystems. From the symmetry point of view, when two subsystems V_1 and V_2 have the same symmetry, which means that they are representations of the same group G, $\rho_1 : G \to GL(V_1)$, $\rho_2 : G \to GL(V_2)$, the composed system $V_1 \otimes V_2$ also has the same symmetry, with symmetry action given by

$$\begin{aligned} \rho : G &\to G \times G \to GL(V_1 \otimes V_2) \\ g &\mapsto (g, g) \mapsto \rho_1(g) \otimes \rho_2(g). \end{aligned}$$

Namely, the symmetry acts on subsystems component-wise. (This is another place that you can modify the most natural structure, as a result you can go beyond group-like symmetries.)

In particular, if we consider a Lie group $\mathrm{e}^{-\mathrm{i}Ar}$ action on both subsystems, whose corresponding conserved quantity is given by the Hermitian generator A, the tensor product action on the composed system is

$$\mathrm{e}^{-\mathrm{i}Ar} \otimes \mathrm{e}^{-\mathrm{i}Ar} = \mathrm{e}^{-\mathrm{i}(A\otimes 1)r}\mathrm{e}^{-\mathrm{i}(1\otimes A)r}.$$

Use the fact that $A \otimes 1$ and $1 \otimes A$ commutes in the tensor product total Hilbert space, we find the Lie group action on the composed system to be

$$\mathrm{e}^{-\mathrm{i}(A\otimes 1+1\otimes A)r}.$$

In other words, the corresponding conserved quantity of the composed system is, in the indexed notation

$$A^{\mathrm{total}} = A^{(1)} + A^{(2)} = A \otimes 1 + 1 \otimes A.$$

This is the rule for addition of momentum, angular momentum, etc.

Problem 5.1.2. Show that the addition of momentum is just the usual addition of numbers.

Problem 5.1.3. Calculate the addition of angular momentum, for two spin 1/2 particles.

1. Pick the $S_z = \frac{1}{2}\hbar\sigma_z$ basis of each particle and write down the tensor product basis of the composed system.

2. The total angular momentum operator is

   $$J_i = S_i \otimes 1 + 1 \otimes S_i.$$

   To find the angular momentum of the composed system, first write down the matrix of

   $$J^2 = \sum_i J_i^2.$$

   Find its eigenvalues and eigenstates. How is the total Hilbert space decomposed according to J^2, i.e. the magnitude of angular momentum?

3. Next, within the eigen subspaces of J^2, find the eigenvalues and eigenstates of J_z.

4. You have obtained four orthogonal states with fixed values of J^2 and J_z, they form a new basis. Write down the matrix transforming from the tensor product basis to this new basis. The basis change matrix elements are just the Clebsch–Gordan (CG) coefficients, for the addition of two spin 1/2's.

5.2 An introductory many-body example

In this section we solve a simple many-body system, whose results motivate the postulate of identical particles. Consider N particles with equal mass m, put on a very large ring. Denote the position and momentum operator of the ith particle by $\hat{x}_i$ and $\hat{p}_i$, with the understanding $i + N = i$. The total Hilbert space is the tensor product of the position space of all particles, spanned by $|x_1\rangle \otimes \cdots \otimes |x_N\rangle$. Think $\hat{x}_i$ and $\hat{p}_i$ as acting on the total Hilbert space (indexed notation), we have commutation relations

$$[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\delta_{ij}, \quad [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0.$$

We also consider a simple quadratic interaction between the particles, a spring connecting each pair of nearest particles. The Hamiltonian is thus

$$H = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} m\omega^2 \sum_{i=1}^{N} (\hat{x}_{i+1} - \hat{x}_i)^2.$$

Using the ideas introduced in previous lectures, it is not hard to solve this system. First, we would seek a new linear combination of operators to simplify the Hamiltonian. Second, notice that the Hamiltonian has the discrete translation symmetry, generated by

$$i \to i + 1,$$

and forming the abstract group $\mathbb{Z}_N$. Thus, we try the operators that are invariant under such translation symmetry

$$X_p = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{\frac{2\pi\mathrm{i}}{N} ip} \hat{x}_i, \quad P_p = \frac{1}{\sqrt{N}} \sum_i \mathrm{e}^{-\frac{2\pi\mathrm{i}}{N} ip} \hat{p}_i.$$

Here, i is the position index and $p = 1, \ldots, N$ (again think $p + N = p$) is the (lattice) momentum index, and we are essentially doing Fourier transform on these discrete indices. Using the equation (the transformation coefficients form a unitary matrix)

$$\sum_{i=1}^{N} \mathrm{e}^{\frac{2\pi\mathrm{i}}{N} ip} = N\delta_{p0},$$

we can compute the new commutation relations

$$[X_p, P_q] = \mathrm{i}\hbar\delta_{pq}, \quad [X_p, X_q] = [P_p, P_q] = 0,$$

which is essentially the same as the old ones. Note that X_p and P_p are not Hermitian. Indeed

$$X_p^\dagger = X_{-p}, \quad P_p^\dagger = P_{-p}.$$

Only when $p = 0$ or $p = N/2$ (for even N) they are Hermitian. We will come to this point later.

The inverse transformation is

$$\hat{x}_i = \frac{1}{\sqrt{N}} \sum_p \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} ip} X_p, \quad \hat{p}_i = \frac{1}{\sqrt{N}} \sum_p \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} ip} P_p.$$

Therefore, the Hamiltonian is

$$\begin{aligned} H &= \frac{1}{2mN} \sum_i \sum_p \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} ip} P_p \sum_q \mathrm{e}^{\frac{2\pi \mathrm{i}}{N} iq} P_q \\ &+ \frac{1}{2N} m\omega^2 \sum_i \sum_p (\mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} p} - 1) \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} ip} X_p \sum_q (\mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} q} - 1) \mathrm{e}^{-\frac{2\pi \mathrm{i}}{N} iq} X_q \\ &= \frac{1}{2m} \sum_p P_p P_{-p} + \frac{1}{2} m\omega^2 \sum_p 2(1 - \cos(\frac{2\pi p}{N})) X_p X_{-p}. \end{aligned}$$

We see that the Hamiltonian is decomposed to the $p, -p$ modes. For simplicity we only consider odd N, so only the $p = 0$ mode is special.

$$H_{p\neq 0} = \frac{1}{2m}(P_p P_{-p} + P_{-p} P_p) + m\omega^2 (1 - \cos(\frac{2\pi p}{N}))(X_p X_{-p} + X_{-p} X_p),$$

$$H_{p=0} = \frac{1}{2m} P_0^2,$$

$$H = \sum_{0<p<N/2} H_p + H_{p=0}.$$

For $0 < p < N/2$ we may further define the Hermitian operators

$$\begin{aligned} X_{p,+} &= \frac{1}{\sqrt{2}}(X_p + X_{-p}) = \sqrt{\frac{2}{N}} \sum_i \hat{x}_i \cos \frac{2\pi}{N} ip, \\ X_{p,-} &= \frac{-\mathrm{i}}{\sqrt{2}}(X_p - X_{-p}) = \sqrt{\frac{2}{N}} \sum_i \hat{x}_i \sin \frac{2\pi}{N} ip, \\ P_{p,+} &= \frac{1}{\sqrt{2}}(P_p + P_{-p}) = \sqrt{\frac{2}{N}} \sum_i \hat{p}_i \cos \frac{2\pi}{N} ip, \\ P_{p,-} &= \frac{\mathrm{i}}{\sqrt{2}}(P_p - P_{-p}) = \sqrt{\frac{2}{N}} \sum_i \hat{p}_i \sin \frac{2\pi}{N} ip. \end{aligned}$$

The only nonzero commutation relations are

$$[X_{p,+}, P_{q,+}] = \mathrm{i}\hbar\delta_{pq}, \quad [X_{p,-}, P_{q,-}] = \mathrm{i}\hbar\delta_{pq}.$$

In other words, we can think $X_{p,\pm}$ and $P_{p,\pm}$ as position and momentum of a new particle labeled by $p, \pm$, whose Hamiltonian is like a simple harmonic oscillator,

$$H_{p\neq 0} = \frac{1}{2m}(P_{p,+}^2 + P_{p,-}^2) + m\omega^2 (1 - \cos(\frac{2\pi p}{N}))(X_{p,+}^2 + X_{p,-}^2),$$

with deformed frequency $\omega_p = \omega\sqrt{2(1-\cos(\frac{2\pi p}{N}))}$. We can then apply the harmonic oscillator solution to these modes. Finally, the many-body system is solved

$$H = \frac{1}{2m}P_0^2 + \sum_{0<p<N/2} \hbar\omega_p(a_{p,+}^\dagger a_{p,+} + a_{p,-}^\dagger a_{p,-} + 1).$$

The first term $\frac{1}{2m}P_0^2$ is just the center of mass kinetic energy, and the following terms are harmonic oscillator modes labeled by the lattice momentum p.

In the above example, we start with a bunch of distinguishable particles, with positions $\hat{x}_i$, but end up with a bunch of indistinguishable particles, whose numbers are given by $a_{p,\pm}^\dagger a_{p,\pm}$ and each carries an energy $\hbar\omega_p$ and a lattice momentum p. As long as we have means to exchange energy with this many-body system (which is inevitable in practice), it is a lot easier to observe the indistinguishable particles, i.e., count their numbers according to energy, than to measure the positions of the distinguishable particles, especially when the number N of degrees of freedom is very large, say of the order of the Avogadro's constant 6×10^{23}. If the Hamiltonian is more general and contains higher order terms than the quadratic ones, the higher order terms give rise to interactions between the harmonic oscillator modes from the quadratic terms.

For the time being, we find, and thus just simply postulate, that the fundamental particles in our world, such as electrons, photons, etc., are indistinguishable, or *identical particles*. The above example provides a possible reason, but currently we do not have the experimental power to check whether there is an underlying, more fundamental quantum system that hosts the fundamental particles as excitations. Nonetheless, the formulation of identical particles must be investigated; fundamental or not, they are necessary for describing a lot of phenomena.

5.3 Identical particle

By identical particles, we mean the eigenstates of the number operator N. We can only count the total number of such particles, but cannot distinguish one from another. Each particle may carry a unit of energy (mass), exhibited by a term NE in the Hamiltonian. Besides, each particle may also carries a unit of some other conserved quantities, such as the momentum. These quantities can be used to label the *modes* of such identical particle, and we also have the number operator N_p for each mode. They commute with each other and sum to the total number

$$[N_p, N_q] = 0, \quad N = \sum_p N_p.$$

Therefore, it is a good, unambiguous way to specify a state of many identical particles, by saying that there are n_p particles with momentum p, n_q particles

with momentum q, etc. These states form the **occupation basis**

$$|n_p, n_q, \ldots\rangle,$$
$$1 = \sum_{n_p, n_q, \ldots} |n_p, n_q, \ldots\rangle\langle n_p, n_q, \ldots|,$$
$$\langle n'_p, n'_q, \ldots | n_p, n_q, \ldots\rangle = \delta_{n_p n'_p}\delta_{n_q n'_q}\cdots.$$
$$N_p|n_p, n_q, \ldots\rangle = n_p|n_p, n_q, \ldots\rangle, \quad N_q|n_p, n_q, \ldots\rangle = n_q|n_p, n_q, \ldots\rangle.$$

We expect the operators $a_p^\dagger$ and a_q to create and annihilate particles in the p, q modes

$$a_p^\dagger|n_p, n_q, \ldots\rangle = C_1|n_p+1, n_q, \ldots\rangle, \quad a_q|n_p, n_q, \ldots\rangle = C_2|n_p, n_q-1, \ldots\rangle,$$

but in general there will be non-zero factors C_1, C_2, including both normalization and phase factors, for us to fix. Note that the occupation basis are also the eigenstates of $a_p^\dagger a_p$ (or $a_p a_p^\dagger$), which means by properly adjusting the normalization factor it is possible to use $a_p^\dagger a_p$ as the number operator. On the other hand, we see that a generic occupation basis state may be expressed in terms of creation operators together with the **vacuum state** $|0\rangle$, i.e., the state with no identical particles,

$$(a_p^\dagger)^{n_p}(a_q^\dagger)^{n_q}\cdots|0\rangle = C|n_p, n_q, \ldots\rangle.$$

Different choices of the normalization and phase factor C correspond to different **statistics** of the identical particle. Currently we know that there can be many non-trivial types of statistics, but here let's discuss the two simplest ones, Bose statistics and Fermi statistics. The identical particles satisfying Bose and Fermi statistics are called *boson* and *fermion*, respectively.

The idea behind the Bose and Fermi statistics is that one may exchange two identical particles, and the resulting state should remain the same, up to an overall factor, since identical particles are indistinguishable. If one further assumes that the overall factor, denoted by θ, does not depend on the detailed exchange path, one concludes that $\theta^2 = 1$, since two exchanges are just the identity. The overall factor may be encoded by the commutation relation of creation operators

$$a_p^\dagger a_q^\dagger = \theta a_q^\dagger a_p^\dagger, \ \theta = \pm 1.$$

Let's study the $\theta = 1$ case, Bose statistics first. In this case the ladder operators for different p, q commutes, so we can just think that different p, q represent different harmonic oscillator modes, and fix the ladder operators as in the harmonic oscillator,

$$a_p^\dagger|n_p, n_q, \ldots\rangle = \sqrt{n_p+1}|n_p+1, n_q, \ldots\rangle, \quad a_q|n_p, n_q, \ldots\rangle = \sqrt{n_q}|n_p, n_q-1, \ldots\rangle,$$

and $N_p = a_p^\dagger a_p$. Alternatively, similar as we have derived in the harmonic oscillator section, the explicit expressions above are equivalent to the commutation relations

$$[a_p, a_q^\dagger] = \delta_{pq}, \quad [a_p, a_q] = 0.$$

The $\theta = -1$, Fermi statistics case, is more involved. Let's study a single mode first, dropping the mode label p. Also to distinguish from the Bose case, we use $c^\dagger, c$ instead of $a^\dagger, a$. The anti-commutation

$$c^\dagger c^\dagger = -c^\dagger c^\dagger$$

implies $c^\dagger c^\dagger = 0$, thus

$$c^\dagger c^\dagger |0\rangle \sim c^\dagger |1\rangle = 0.$$

In other words, the occupation number for fermions can only be 0 or 1. There are only two states, we can simply fix

$$c|0\rangle = c^\dagger |1\rangle = 0, \quad c|1\rangle = |0\rangle, \quad c^\dagger |0\rangle = |1\rangle.$$

Then it is not hard to check $c^\dagger c = N$ is the number operator. Similar to the boson case, these explicit expressions are equivalent to the anti-commutation relations

$$\{c_p, c_q^\dagger\} = \delta_{pq}, \quad \{c_p, c_q\} = 0.$$

The anti-commutator is defined as $\{A, B\} = AB + BA$.

Problem 5.3.1. Use $\{c, c^\dagger\} = 1, \{c, c\} = 0$ to derive the commutation relations

$$[c^\dagger c, c^\dagger] = c^\dagger, \quad [c^\dagger c, c] = -c,$$

which means that $c^\dagger$ increases and c decreases the eigenvalue of $c^\dagger c$ by 1.

Since c_p and c_q for different modes anti-commutes, the order of the ladder operators matters and could contribute a non-trivial sign. We have to fix an order when express the occupation basis using the creation operators, for example

$$|n_p, n_q\rangle = (c_p^\dagger)^{n_p} (c_q^\dagger)^{n_q} |0\rangle.$$

In the above convention, the sign of the creation operator $c_q^\dagger$ for the second mode depends on whether the first mode is occupied,

$$c_q^\dagger |0, 0\rangle = |0, 1\rangle, \quad c_q^\dagger |1, 0\rangle = -|1, 1\rangle.$$

5.4 Field operator

For identical particles, it is no longer sound to speak about the position of a specific particle. In this section we inspect the proper way to describe the positions of many identical particles, using field operators, and also discuss the many-body Hamiltonian.

When there is only one identical particle, we can identify its state with a single particle state. We consider Bose statistics first. For momentum p, it means

$$a_p^\dagger |0\rangle = |p\rangle.$$

However, $a_p^\dagger a_q^\dagger|0\rangle$ is not, for example, the tensor product $|p\rangle \otimes |q\rangle$. Think about why.

Let $\psi^\dagger(x)$ be the **operator** that creates a particle at position x, namely,

$$\psi^\dagger(x)|0\rangle = |x\rangle.$$

$\psi^\dagger(x)$ is the so-called *field operator*. It is a bunch of operators **indexed** by the position x. We can now associate the single particle wavefunction to the operators

$$\langle 0|\psi(x)a_p^\dagger|0\rangle = \langle x|p\rangle.$$

For simplicity, let's assume that the momentum exhausts the possible degrees of freedom of our identical particles, which means that we should be able to express $\psi(x)$ as a linear combination of the momentum annihilation operator,

$$\psi(x) = \sum_p \varphi_{px} a_p.$$

We then find

$$\begin{aligned}\langle x|p\rangle = \langle 0|\psi(x)a_p^\dagger|0\rangle &= \langle 0|\sum_q \varphi_{qx} a_q a_p^\dagger|0\rangle \\ &= \langle 0|\sum_q \varphi_{qx}(\delta_{pq} + a_p^\dagger a_q)|0\rangle = \varphi_{px}.\end{aligned}$$

Here and later we may leave the form of $\langle x|p\rangle$ implicit for application in similar scenarios:

1. x, p are both continuous.
2. x is finite but continuous while p is discrete (box normalization).
3. p is finite but continuous while x is discrete (discrete translation symmetry).
4. x, p are both discrete, as the example in the previous section.

The matrix elements $\langle x|p\rangle = \varphi_{px}$ are all of similar exponential forms, only with different normalizations. As the box normalization is new to us, we discuss it briefly and will use the notation for continuous x but discrete p.

As the name indicates, box normalization means that we restrict the position within a finite box, say of length L. If you like, you may later let $L \to \infty$ to recover the x, p both continuous case. It is more convenient to impose the periodic boundary condition $|x\rangle = |x + L\rangle$ (so that for 1-dimensional system it is a ring, for 2-dimensional system it is a torus, for 3-dimensional system it is a 3-torus, which is hard to imagine and that is why people just say box normalization). The momentum becomes quantized due to the constraint

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px} \sim \langle x|p\rangle = \langle x + L|p\rangle \sim \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x+L)},$$

thus

$$\mathrm{e}^{\frac{\mathrm{i}}{\hbar}pL} = 1, \quad p = \frac{2\pi\hbar}{L}k,\ k \in \mathbb{Z}.$$

And the normalization is

$$\delta_{pq} = \langle q|p\rangle = \int_0^L \mathrm{d}x\, \langle q|x\rangle\langle x|p\rangle, \tag{5.1}$$

which leads to

$$\langle x|p\rangle = \frac{1}{\sqrt{L}}\mathrm{e}^{\frac{\mathrm{i}}{\hbar}px}.$$

Due to the Fourier expansion theorem for periodic functions $f(x) = f(x+L)$,

$$f(x) = \sum_k c_k \frac{1}{\sqrt{L}}\mathrm{e}^{\frac{2\pi\mathrm{i}}{L}kx}, \quad c_k = \int_0^L \mathrm{d}y\, f(y)\frac{1}{\sqrt{L}}\mathrm{e}^{-\frac{2\pi\mathrm{i}}{L}ky},$$

we have

$$\delta(x-y) = \sum_k \frac{1}{L}\mathrm{e}^{\frac{2\pi\mathrm{i}}{L}k(x-y)} = \sum_p \langle x|p\rangle\langle p|y\rangle. \tag{5.2}$$

This formula also helps us to get the $L \to \infty$ limit. When $L \to \infty$, $p = \frac{2\pi\hbar}{L}k$ becomes continuous and we should identify $\mathrm{d}p = \frac{2\pi\hbar}{L}$, therefore

$$\int \mathrm{d}p \sim \sum_k \frac{2\pi\hbar}{L},$$

$$\lim_{L\to\infty} \sum_k \frac{1}{L} = \int \frac{\mathrm{d}p}{2\pi\hbar}.$$

We recover the normalization of delta function for continuous p

$$\delta(x-y) = \frac{1}{2\pi\hbar}\int \mathrm{d}p\, \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}.$$

Now for the field operator

$$\psi(x) = \sum_p \langle x|p\rangle a_p, \quad \psi^\dagger(x) = \sum_p a_p^\dagger \langle p|x\rangle,$$

using the the unitarity (5.1)(5.2) of $\langle x|p\rangle$, we have the commutation relations

$$[\psi(x), \psi^\dagger(y)] = \delta(x-y), \quad [\psi(x), \psi(y)] = 0,$$

and inverse transform

$$a_p = \int_0^L \mathrm{d}x\, \langle p|x\rangle\psi(x), \quad a_p^\dagger = \int_0^L \mathrm{d}x\, \psi^\dagger(x)\langle x|p\rangle.$$

Also, the total number of particles

$$N = \sum_p N_p = \sum_p a_p^\dagger a_p = \int_0^L \mathrm{d}x\, \psi^\dagger(x)\psi(x).$$

In the continuous case, $\rho(x) := \psi^\dagger(x)\psi(x)$ is the number *density* operator ($\rho(x)\mathrm{d}x$ is the number operator in the small interval $[x, x+\mathrm{d}x]$), and

$$[\psi^\dagger(x)\psi(x), \psi^\dagger(y)] = \delta(x-y)\psi^\dagger(y),$$

which means that $\psi^\dagger(y)$ increases the density by $\delta(x-y)$, and

$$[N = \int \mathrm{d}x\, \psi^\dagger(x)\psi(x), \psi^\dagger(y)] = \psi^\dagger(y),$$

the total number is increased by 1. Therefore, $\psi^\dagger(y)$ indeed creates a particle at y, whose density is $\delta(x-y)$. Now,

$$|x_1, \ldots, x_n\rangle := \psi^\dagger(x_1)\cdots\psi^\dagger(x_n)|0\rangle$$

is a state with n identical particles at positions $x_1, \ldots, x_n$. We will elaborate on this point later.

Having clarified the unitary transformation between momentum and position field operators, we are ready to write down some commonly seen Hamiltonian terms. Depending on the number of particles involved in the interactions, we may write

$$H = H_0 + H_1 + H_2 + \ldots$$

H_0 is the free part, the kinetic energy, H_1 is the single particle potential energy and H_2 is the two-body interaction, etc. The kinetic energy H_0 is diagonal in the momentum occupation basis

$$H_0 = \sum_p \frac{p^2}{2m} N_p = \sum_p \frac{p^2}{2m} a_p^\dagger a_p.$$

In the position basis

$$H_0 = \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \sum_p \frac{1}{L}\frac{p^2}{2m} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)} \psi^\dagger(x)\psi(y).$$

Note that

$$\frac{\partial^2}{\partial y^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)} = -\frac{p^2}{\hbar^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}.$$

We may sum over p first and then take the above partial derivative

$$\begin{aligned}
H_0 &= \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \sum_p \frac{1}{L}\frac{p^2}{2m} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)} \psi^\dagger(x)\psi(y) \\
&= \int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \sum_p -\frac{1}{L}\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial y^2} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}\right) \psi^\dagger(x)\psi(y) \\
&= \int_0^L \mathrm{d}x\, \psi^\dagger(x) \int_0^L \mathrm{d}y \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} \sum_p \frac{1}{L} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}p(x-y)}\right) \psi(y) \\
&= \int_0^L \mathrm{d}x\, \psi^\dagger(x) \int_0^L \mathrm{d}y \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} \delta(x-y)\right) \psi(y).
\end{aligned}$$

To evaluate the integral with respect to y, we are going to use integration by parts repeatedly. Note that we have a integral with respect to x in front, and the boundary terms $x = 0$ and $x = L$ occupy only a zero length (zero measure) comparing to the whole interval $[0, L]$, so we can think $0 < x < L$ while integration by parts, with

$$\delta(x-y)\Big|_{y=0,y=L} = \frac{\partial}{\partial y}\delta(x-y)\Big|_{y=0,y=L} = \frac{\partial^2}{\partial y^2}\delta(x-y)\Big|_{y=0,y=L} = 0.$$

Therefore,

$$\begin{aligned}
&\int_0^L \mathrm{d}y \left(\frac{\partial^2}{\partial y^2}\delta(x-y)\right)\psi(y) \\
&= \psi(y)\frac{\partial}{\partial y}\delta(x-y)\Big|_{y=0}^{y=L} - \int_0^L \mathrm{d}y \left(\frac{\partial}{\partial y}\delta(x-y)\right)\frac{\partial}{\partial y}\psi(y) \\
&= -\delta(x-y)\frac{\partial}{\partial y}\psi(y)\Big|_{y=0}^{y=L} + \int_0^L \mathrm{d}y\, \delta(x-y)\frac{\partial^2}{\partial y^2}\psi(y) \\
&= \frac{\partial^2}{\partial x^2}\psi(x).
\end{aligned}$$

Finally we have

$$H_0 = \int \mathrm{d}x\, \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x).$$

The above derivation involving integral transform also works for single particle states $|x\rangle, |p\rangle$, that is why we got the same form $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ for kinetic energy.

The single particle potential energy H_1 is diagonal in the position occupation basis

$$H_1 = \int \mathrm{d}x\, V_1(x)\rho(x) = \int \mathrm{d}x\, \psi^\dagger(x)V_1(x)\psi(x).$$

In the momentum basis,

$$H_1 = \sum_{p,q}\int \mathrm{d}x\, \langle p|x\rangle a_p^\dagger V_1(x)\langle x|q\rangle a_q = \sum_{p,q} V_{pq}a_p^\dagger a_q,$$

where the Fourier transform of the potential

$$V_{pq} = \int \mathrm{d}x\, \langle p|x\rangle V_1(x)\langle x|q\rangle,$$

needs to be calculated or given on a case by case basis.

We consider the two-body interaction H_2 given by some two-body potential $V_2(x, y) = V_2(y, x)$ (for example, the Coulomb potential) which is diagonal in the two-body position states $|x, y\rangle$. Classically, the two-body energy is given by the integration of the two-body potential $V_2(x, y)$ times the densities $\rho(x)$ and

$\rho(y)$ at x and y, divided by 2 as we counted twice for each pair of positions. Naive quantization gives

$$\begin{aligned}&\frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y\, V_2(x,y)\rho(x)\rho(y)\\ &= \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y\, V_2(x,y)\psi^\dagger(x)\psi(x)\psi^\dagger(y)\psi(y).\end{aligned}$$

You can easily verify $[\rho(x),\rho(y)]=0$ so their order does not matter. However, the correct quantization is to use the *normal order* of field operators, that is putting all creation operators to the left and all annihilation operators to the right. In the normal order convention

$$\begin{aligned}H_2 &= \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y\, \psi^\dagger(x)\psi^\dagger(y)V_2(x,y)\psi(y)\psi(x)\\ &= \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y\, \psi^\dagger(x)\psi(x)V_2(x,y)\psi^\dagger(y)\psi(y) - \frac{1}{2}\int \mathrm{d}x\, \psi^\dagger(x)V_2(x,x)\psi(x).\end{aligned}$$

The difference is a nontrivial modification $\frac{1}{2}V_2(x,x)$ to the single particle potential. To see why the normal order is the correct one, remember the fundamental philosophy of measurement. The two-body potential $V_2(x,y)$ should be measured by the energy of a two-body state

$$H_2|x,y\rangle = V_2(x,y)|x,y\rangle,$$

where $|x,y\rangle = \psi^\dagger(x)\psi^\dagger(y)|0\rangle$. Now insert H_2 and perform the calculation

$$H_2|x,y\rangle = \frac{1}{2}\iint \mathrm{d}u\mathrm{d}v\, \psi^\dagger(u)\psi^\dagger(v)V_2(u,v)\psi(v)\psi(u)\psi^\dagger(x)\psi^\dagger(y)|0\rangle.$$

Let's focus on the rightmost part

$$\begin{aligned}\psi(v)\psi(u)\psi^\dagger(x)\psi^\dagger(y)|0\rangle &= \psi(v)\left(\delta(u-x)+\psi^\dagger(x)\psi(u)\right)\psi^\dagger(y)|0\rangle\\ &= \delta(u-x)\delta(v-y)|0\rangle + \delta(v-x)\delta(u-y)|0\rangle,\end{aligned}$$

where we have used $\psi(u)|0\rangle = \psi(v)|0\rangle = 0$. Thus,

$$\begin{aligned}&H_2|x,y\rangle\\ &= \frac{1}{2}\iint \mathrm{d}u\mathrm{d}v\, \psi^\dagger(u)\psi^\dagger(v)V_2(u,v)\left(\delta(u-x)\delta(v-y)+\delta(v-x)\delta(u-y)\right)|0\rangle\\ &= \frac{1}{2}\left(\psi^\dagger(x)\psi^\dagger(y)V_2(x,y)|0\rangle + \psi^\dagger(y)\psi^\dagger(x)V_2(y,x)|0\rangle\right)\\ &= V_2(x,y)|x,y\rangle,\end{aligned}$$

as desired. Also, it is easy to compute

$$\frac{1}{2}\int \mathrm{d}u\, \psi^\dagger(u)V_2(u,u)\psi(u)|x,y\rangle = \frac{1}{2}(V_2(x,x)+V_2(y,y))|x,y\rangle,$$

which means that the naive quantization overcounts the self-interaction

$$\frac{1}{2}V_2(x,x)+\frac{1}{2}V_2(y,y).$$

It is then straightforward to transform into the momentum basis

$$H_2=\frac{1}{2}\sum_{p,q,r,s}V_{pqrs}a_p^\dagger a_q^\dagger a_r a_s,$$

where

$$V_{pqrs}=\iint \mathrm{d}x\mathrm{d}y\,\langle p|x\rangle\langle q|y\rangle V_2(x,y)\langle y|r\rangle\langle x|s\rangle.$$

The story is completely similar for fermions. For fermion creation and annihilation operators $c_p^\dagger, c_p$, with anti-commutation relations

$$\{c_p,c_q^\dagger\}=\delta_{pq},\ \{c_p,c_q\}=0,$$

We still define fermionic field operators

$$\psi(x)=\sum_p\langle x|p\rangle c_p.$$

They have anti-commutation relations

$$\{\psi(x),\psi^\dagger(y)\}=\delta(x-y),\quad \{\psi(x),\psi(y)\}=0.$$

The number operators and Hamiltonian terms we discussed, are of the same form as bosons. The only thing to be careful with is the normal order for interactions between two or more. For fermions, the order of positions needs to be reversed between creation and annihilation operators. Though it makes no difference for bosons, it is recommended to always follow such rule.

Problem 5.4.1. For fermionic field operators

$$\psi(x)=\sum_p\langle x|p\rangle c_p,$$

and two-body interaction

$$H_2=\frac{1}{2}\int \mathrm{d}x\int \mathrm{d}y\,\psi^\dagger(x)\psi^\dagger(y)V_2(x,y)\psi(y)\psi(x),$$

verify again

$$H_2\psi^\dagger(x)\psi^\dagger(y)|0\rangle=V_2(x,y)\psi^\dagger(x)\psi^\dagger(y)|0\rangle.$$

Also compute the difference between the normal order and the naive quantization

$$\frac{1}{2}\int \mathrm{d}x\int \mathrm{d}y\,V_2(x,y)\rho(x)\rho(y).$$

Be careful about the signs and learn how they cancel up to give the same form of result as the bosonic case.

5.5 Many-body wavefunction

We finish the many-body theory part by discussing the many-body wavefunction. Naively, for an n-body state $|\Psi\rangle$, the wavefunction is just

$$\langle x_1, \ldots, x_n|\Psi\rangle.$$

It has some nontrivial properties with respect to permutation and normalization. Traditionally, these properties are attributed to the wavefunction; however, a probably better view is to attribute them to the position basis

$$|x_1, \ldots, x_n\rangle := \psi^\dagger(x_1)\cdots\psi^\dagger(x_n)|0\rangle,$$

and in turn to the algebraic relations of the field operator $\psi(x)$.

The permutation property is relatively easy. When two positions are exchanged, we get a minus sign for fermions and nothing for bosons. As an example, suppose we exchange x_1 and x_n for fermions

$$\begin{aligned}
&\psi^\dagger(x_1)\cdots\psi^\dagger(x_n) = (-1)^{n-1}\psi^\dagger(x_2)\cdots\psi^\dagger(x_n)\psi^\dagger(x_1)\\
&= (-1)^{n-1}(-1)^{n-2}\psi^\dagger(x_n)\psi^\dagger(x_2)\cdots\psi^\dagger(x_{n-1})\psi^\dagger(x_1)\\
&= -\psi^\dagger(x_n)\psi^\dagger(x_2)\cdots\psi^\dagger(x_{n-1})\psi^\dagger(x_1).
\end{aligned}$$

The normalization is slightly nontrivial. For simplicity, let's consider the discrete momentum modes first. The occupation states

$$|n_{p_1}, n_{p_2}, \ldots\rangle,$$

form an orthonormal basis, provided that we choose a fixed order of the momentum indices $p_1, p_2, \ldots$,

$$1 = \sum_{n_{p_1}, n_{p_2}, \ldots} |n_{p_1}, n_{p_2}, \ldots\rangle\langle n_{p_1}, n_{p_2}, \ldots|.$$

The total number of particles is not fixed; the above way of decomposing the identity is like the *grand canonical ensemble*. But we may as well do it in the *canonical ensemble* way. The total number operator N surely is a Hermitian observable. States with different total numbers of particles form different eigensubspaces of N and have mutually no overlap. Denote by P_n the projection to the n-particle state

$$P_n = \sum_{n_{p_1}+n_{p_2}+\cdots=n} |n_{p_1}, n_{p_2}, \ldots\rangle\langle n_{p_1}, n_{p_2}, \ldots|,$$

and

$$1 = \sum_{n=0}^{\infty} P_n.$$

As you can see, the occupation basis is no longer convenient when the total number of particles is fixed. But it is easy to see that you need a fixed number

of creation operators acting on the vacuum state to obtain a state with fixed total number of particles. So instead, it is better to just specify the momenta $p_1, \ldots, p_n$ of n particles, and define the n-body state

$$|p_1, \ldots, p_n\rangle := a^\dagger_{p_1} \cdots a^\dagger_{p_n} |0\rangle.$$

However, the normalization becomes nontrivial. When all $p_1, \ldots, p_n$ are different, the above state is normalized. But when some of $p_1, \ldots, p_n$ are the same, for example $p_1 = p_2 = p_3 < p_4 < \cdots < p_n$, we know

$$\begin{aligned} &|n_{p_1} = 3, n_{p_4} = 1, \ldots, n_{p_n} = 1, \text{ other } n_p = 0\rangle \\ &= \frac{(a^\dagger_{p_1})^3}{\sqrt{3!}} a^\dagger_{p_4} \cdots a^\dagger_{p_n} |0\rangle \\ &= \frac{1}{\sqrt{3!}} |p_1 = p_2 = p_3, p_4, \ldots, p_n\rangle, \end{aligned}$$

is normalized. Therefore,

$$P_n = \left(\sum_{p_1 < \cdots < p_n} + \frac{1}{2!} \sum_{p_1 = p_2 < p_3 < \cdots < p_n} + \cdots \right) |p_1, \ldots, p_n\rangle\langle p_1, \ldots, p_n|.$$

Surely such subtlety vanishes for fermions. It also gets simplified for continuous modes, since except the first summation, all remaining summations are over zero area, volume or hyper-volume (zero measure) and thus negligible. Therefore, it is preferred to consider n-particle states in terms of continuous modes, for example the continuous position in box normalization:

$$P_n = \int_0^L \mathrm{d}x_1 \int_{x_1}^L \mathrm{d}x_2 \cdots \int_{x_{n-1}}^L \mathrm{d}x_n \, |x_1, \ldots, x_n\rangle\langle x_1, \ldots, x_n|.$$

It looks better to use uniform interval for all the positions and then correct for the overcounting. It is clear that any permutation of $x_1, \ldots, x_n$ gives the same state as $|x_1, \ldots, x_n\rangle$, at most up to a sign for fermions, and exactly the same projection $|x_1, \ldots, x_n\rangle\langle x_1, \ldots, x_n|$. Thus we are overcounting $n!$ times,

$$P_n = \frac{1}{n!} \int_0^L \mathrm{d}x_1 \cdots \int_0^L \mathrm{d}x_n \, |x_1, \ldots, x_n\rangle\langle x_1, \ldots, x_n|,$$

and this is where the mysterious factor $1/n!$ arises. For a normalized n-body state $|\Psi\rangle$,

$$\begin{aligned} 1 = \langle\Psi|\Psi\rangle &= \langle\Psi|P_n|\Psi\rangle \\ &= \frac{1}{n!} \int \mathrm{d}x_1 \cdots \mathrm{d}x_n \, \langle\Psi|x_1, \ldots, x_n\rangle\langle x_1, \ldots, x_n|\Psi\rangle \\ &= \int \mathrm{d}x_1 \cdots \mathrm{d}x_n \left| \frac{1}{\sqrt{n!}} \langle x_1, \ldots, x_n|\Psi\rangle \right|^2. \end{aligned}$$

Although conventionally, as many textbooks do, people put $1/\sqrt{n!}$ together with $\langle x_1, \ldots, x_n|\Psi\rangle$ and call

$$\frac{1}{\sqrt{n!}}\langle x_1, \ldots, x_n|\Psi\rangle$$

the normalized many-body wavefunction, the factor $1/\sqrt{n!}$ in fact comes from overcounting the position basis states in the resolution of identity.

We have finished introducing the basic formulism of many-body physics. A good way to memorize them is the idea of "second quantization". Recall that in the canonical quantization, a key procedure is to replace numbers by operators. "Second quantization" is in fact better termed "second operatorization". We are not quantizing again; the many-body theory is already a quantum theory from the very beginning. However, there is indeed an analog between single-body quantum mechanics and many-body quantum mechanics, by replacing numbers by operators, for example as listed in Table 5.1.

Single-body	Many-body
wavefunction $\psi(x) = \langle x|\psi\rangle$	field operator $\psi(x)$
probability density $\psi^*(x)\psi(x)$	density operator $\psi^\dagger(x)\psi(x)$
kinetic energy expectation value $\langle\psi|\frac{\hat{p}^2}{2m}|\psi\rangle = \int \mathrm{d}x\, \psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x)$	kinetic energy operator $\int \mathrm{d}x\, \psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\psi(x)$
potential energy expectation value $\langle\psi|V(\hat{x})|\psi\rangle = \int \mathrm{d}x\, \psi^*(x)V(x)\psi(x)$	potential energy operator $\int \mathrm{d}x\, \psi^\dagger(x)V(x)\psi(x)$

Table 5.1: Second quantization correspondence.

It is helpful to compute the expectation values in many-body theory. Again assuming $|\Psi\rangle$ an n-body state, we compute for example the expectation of density

$$\begin{aligned}\langle\Psi|\psi^\dagger(x)\psi(x)|\Psi\rangle &= \frac{1}{n!}\int \mathrm{d}x_1 \cdots \mathrm{d}x_n \langle\Psi|\psi^\dagger(x)\psi(x)|x_1, \ldots, x_n\rangle\langle x_1, \ldots, x_n|\Psi\rangle \\ &= \frac{1}{n!}\int \mathrm{d}x_1 \cdots \mathrm{d}x_n \langle\Psi|\psi^\dagger(x)\psi(x)\psi^\dagger(x_1)\cdots\psi^\dagger(x_n)|0\rangle\langle x_1, \ldots, x_n|\Psi\rangle.\end{aligned}$$

Let's focus on

$$\begin{aligned}&\psi(x)\psi^\dagger(x_1)\cdots\psi^\dagger(x_n) \\ &= \Big(\delta(x - x_1) \pm \psi^\dagger(x_1)\psi(x)\Big)\psi^\dagger(x_2)\cdots\psi^\dagger(x_n) \\ &= \sum_{j=1}^{n}(\pm)^{j-1}\psi^\dagger(x_1)\cdots\psi^\dagger(x_{j-1})\delta(x - x_j)\psi^\dagger(x_{j+1})\cdots\psi^\dagger(x_n) \\ &+ (\pm)^n\psi^\dagger(x_1)\cdots\psi^\dagger(x_n)\psi(x).\end{aligned}$$

Here we are dealing with bosons and fermions on equal footing by keeping the sign $(\pm)$. The last term acting on $|0\rangle$ leads to zero. For the jth term, integration

with respect to x_j sets x_j to x, and moving $\psi^\dagger(x)$ to the jth position generates the same sign $(\pm)^{j-1}$. Therefore,

$$\begin{aligned}&\langle\Psi|\psi^\dagger(x)\psi(x)|\Psi\rangle\\&=\frac{1}{n!}\sum_{j=1}^{n}\int \mathrm{d}x_1\cdots\mathrm{d}x_{j-1}\mathrm{d}x_{j+1}\cdots\mathrm{d}x_n|\langle x_1,\ldots,x_{j-1},x,x_{j+1},\ldots,x_n|\Psi\rangle|^2.\end{aligned}$$

As a consistent check, we may further integrate with respect to x to get the total number of particles, which has to be n. Using the normalization of $|\Psi\rangle$ we indeed find

$$\begin{aligned}&\langle\Psi|\int \mathrm{d}x\,\psi^\dagger(x)\psi(x)|\Psi\rangle\\&=\sum_{j=1}^{n}\frac{1}{n!}\int \mathrm{d}x_1\cdots\mathrm{d}x_{j-1}\mathrm{d}x\mathrm{d}x_{j+1}\cdots\mathrm{d}x_n|\langle x_1,\ldots,x_{j-1},x,x_{j+1},\ldots,x_n|\Psi\rangle|^2.\\&=\sum_{j=1}^{n}1=n.\end{aligned}$$

Problem 5.5.1. 1. For a bosonic two-body state with fixed momenta p_1, p_2

$$|p_1,p_2\rangle=a^\dagger_{p_1}a^\dagger_{p_2}|0\rangle,$$

express the two-body wavefunction

$$\frac{1}{\sqrt{2!}}\langle x_1,x_2|p_1,p_2\rangle$$

in terms of single particle wavefunction $\langle x|p\rangle$. Check the normalization using the single particle orthonormal property

$$\int \mathrm{d}x\,\langle q|x\rangle\langle x|p\rangle=\delta_{pq},$$

for both $p_1\neq p_2$ and $p_1=p_2$.

2. Repeat the above for a fermionic two-body state

$$|p_1,p_2\rangle=c^\dagger_{p_1}c^\dagger_{p_2}|0\rangle.$$

3. For fermionic n-body states

$$|p_1,\ldots,p_n\rangle:=c^\dagger_{p_1}\cdots c^\dagger_{p_n}|0\rangle,$$

prove its normalization

$$\langle q_1,\ldots,q_n|p_1,\ldots,p_n\rangle=\det(\delta_{q_ip_j}),$$

by explicitly evaluating the anti-commutation of creation and annihilation operators, and induction on n. Here $(\delta_{q_i p_j})$ denotes a matrix whose (i,j) entry is $\delta_{q_i p_j}$. You may use the Laplace expansion (inductive expansion) of determinant

$$\det A = \sum_i (-1)^{i+j} A_{ij} \det A_{\widetilde{ij}},$$

where A_{ij} is the (i,j) entry of A and $A_{\widetilde{ij}}$ is the matrix obtained by deleting the i-th row and j-th column of A.

4. Based on the above result, evaluate the normalization

$$\langle q_1, \ldots, q_n | p_1, \ldots, p_n \rangle$$

for bosonic states and

$$\langle y_1, \ldots, y_n | x_1, \ldots, x_n \rangle$$

for both fermionic and bosonic states.

Hint: The determinant can be written in terms of permutations,

$$\det A = \det(A_{ij}) = \sum_{\sigma \in S_n} \operatorname{sgn} \sigma \prod_{i=1}^{n} A_{i\sigma(i)}.$$

Here, S_n is the set of all invertible maps between

$$\{1, 2, \ldots, n\} \to \{1, 2, \ldots, n\},$$

namely, S_n is the permutation group of n elements. $\forall \sigma \in S_n$,

$$\sigma(1), \sigma(2), \ldots, \sigma(n)$$

is a permutation of $1, 2, \ldots, n$. Every permutation can be expressed as the composition of transpositions (a transposition is an exchange of two elements with all others staying the same). Such expression may not be unique; however, let the number of transpositions be k, then the parity $\operatorname{sgn} \sigma = (-1)^k$ is an invariant for a given permutation σ. For example,

$$c_{p_n} \cdots c_{p_1} = (\operatorname{sgn} \sigma) c_{p_{\sigma(n)}} \cdots c_{p_{\sigma(1)}}.$$

5. Find the general expression in terms of single particle wavefunction of the n-body wavefunction

$$\frac{1}{\sqrt{n!}} \langle x_1, \ldots, x_n | p_1, \ldots, p_n \rangle,$$

for both bosons and fermions.

Chapter 6

Perturbation and Scattering Theory

6.1 Non-degenerate perturbation theory

Consider a Hamiltonian $H(\lambda)$ that depends on a parameter λ. Suppose at $\lambda = 0$ all the energy eigenstates are not degenerate, thus up to a phase factor, we have a well-defined orthonormal basis $|n(0)\rangle$, distinguishable by their energy $H(0)|n(0)\rangle = E_n(0)|n(0)\rangle$. When λ is varied a little bit, and the energy levels $E_n(\lambda)$ are also not changed a lot, namely $|E_n(\lambda) - E_n(0)| \ll \min |E_m(0) - E_n(0)|$, the energy eigenstates will remain non-degenerate, and we should still have a well-defined orthogonal basis $|n(\lambda)\rangle$. To fix the phase factor choice at different λ, also for later convenience, we choose the normalization convention

$$\langle n(0)|n(\lambda)\rangle = 1.$$

Our goal is to solve

$$H(\lambda)|n(\lambda)\rangle = E_n(\lambda)|n(\lambda)\rangle.$$

The idea behind a perturbative solution is as follows. Suppose that we want to determine an unknown function $f(x)$, which is a combination of several unknown functions and satisfies

$$f(x) = 0,$$

in a small neighborhood $x \in (-\epsilon, \epsilon)$ around 0. It is impossible to solve it at every point; instead, one expands $f(x)$ to the power series

$$0 = f(x) = f(0) + f^{(1)}(0)x + \frac{1}{2}f^{(2)}(0)x^2 + \frac{1}{6}f^{(3)}(0)x^3 + \dots$$

and requires the coefficients of x^n to be zero, namely $f^{(n)}(0) = 0$. For x small enough, a good approximate solution can be obtained from the first several orders of equations. In practice, $f(x)$ may be the sum, product or composition

of other functions; depending on situations, sometimes it is more convenient to first expand these functions to proper orders and then compute the sum, product or composition of the resulting polynomials. Here for the formal derivation of the formulas, we instead choose to take derivatives iteratively. Also, the generalization to multiple parameters is straightforward; we will use the shorthand notation

$$\partial_\nu f(x^\mu) := \frac{\partial f}{\partial x^\nu}(x^\mu),$$

and the convention that a function without explicit variable is to be evaluated at 0

$$f := f(x^\mu)\Big|_{x^\mu=0}, \quad \partial_\mu f := \frac{\partial f}{\partial x^\mu}(x^\nu)\Big|_{x^\nu=0}.$$

Now, for a Hamiltonian $H(x^\mu)$ depending on several parameters x^μ, we want to solve

$$(E_n(x^\mu) - H(x^\mu))|n(x^\mu)\rangle = 0.$$

The zeroth order equation is

$$H|n\rangle = E_n|n\rangle.$$

We assume throughout this section that $E_n \neq E_m$ for $n \neq m$, and $|n\rangle$ form an orthonormal basis $1 = \sum_n |n\rangle\langle n|$, $\langle m|n\rangle = \delta_{mn}$.

The first derivative is

$$(\partial_\nu E_n(x^\mu) - \partial_\nu H(x^\mu))|n(x^\mu)\rangle + (E_n(x^\mu) - H(x^\mu))|\partial_\nu n(x^\mu)\rangle = 0.$$

The function equation should be kept as it is if higher orders are to be calculated. Setting $x^\mu = 0$ we obtain the first order equation

$$(\partial_\nu E_n - \partial_\nu H)|n\rangle + (E_n - H)|\partial_\nu n\rangle = 0. \tag{6.1}$$

Our normalization convention is

$$\langle n|n(x^\mu)\rangle = 1,$$

which implies $\langle n|\partial_\mu \cdots \partial_\nu n\rangle = 0$. Thus by projecting (6.1) to $\langle n|$ we obtain the first order energy correction

$$\partial_\nu E_n = \langle n|\partial_\nu H|n\rangle.$$

By projecting (6.1) to $\langle m|$, $m \neq n$, we obtain the first order state correction

$$(E_n - E_m)\langle m|\partial_\nu n\rangle = \langle m|\partial_\nu H|n\rangle,$$

namely

$$|\partial_\nu n\rangle = \sum_{m\neq n} |m\rangle \frac{\langle m|\partial_\nu H|n\rangle}{E_n - E_m}.$$

The second order equation is

$$\begin{aligned}&(\partial_\mu\partial_\nu E_n - \partial_\mu\partial_\nu H)|n\rangle + (E_n - H)|\partial_\mu\partial_\nu n\rangle \\ &+ (\partial_\mu E_n - \partial_\mu H)|\partial_\nu n\rangle + (\partial_\nu E_n - \partial_\nu H)|\partial_\mu n\rangle = 0. \end{aligned} \tag{6.2}$$

Again, project (6.2) to $\langle n|$ and we obtain

$$\partial_\mu\partial_\nu E_n - \langle n|\partial_\mu\partial_\nu H|n\rangle - \langle n|\partial_\mu H|\partial_\nu n\rangle - \langle n|\partial_\nu H|\partial_\mu n\rangle = 0.$$

Using the result of $|\partial_\nu n\rangle$ we obtain the second order energy correction

$$\partial_\mu\partial_\nu E_n = \langle n|\partial_\mu\partial_\nu H|n\rangle + \sum_{m\neq n} \frac{\langle n|\partial_\mu H|m\rangle\langle m|\partial_\nu H|n\rangle + \langle n|\partial_\nu H|m\rangle\langle m|\partial_\mu H|n\rangle}{E_n - E_m}.$$

Project (6.2) to $\langle m|$, $m \neq n$ and we obtain

$$\begin{aligned}&\langle m|\partial_\mu\partial_\nu H|n\rangle + (E_n - E_m)\langle m|\partial_\mu\partial_\nu n\rangle \\ &+ \langle m|(\partial_\mu E_n - \partial_\mu H)|\partial_\nu n\rangle + \langle m|(\partial_\nu E_n - \partial_\nu H)|\partial_\mu n\rangle = 0\end{aligned}$$

Substituting $\partial_\mu E_n$ and $|\partial_\mu n\rangle$ we obtain the second order state correction

$$\begin{aligned}|\partial_\mu\partial_\nu n\rangle = &\sum_{m\neq n} |m\rangle \frac{\langle m|\partial_\mu\partial_\nu H|n\rangle}{E_n - E_m} \\ &+ \sum_{m\neq n} |m\rangle \sum_{k\neq n} \frac{\langle m|\partial_\mu H|k\rangle\langle k|\partial_\nu H|n\rangle}{(E_n - E_m)(E_n - E_k)} - \sum_{m\neq n} |m\rangle \frac{\langle n|\partial_\mu H|n\rangle\langle m|\partial_\nu H|n\rangle}{(E_n - E_m)^2} \\ &+ \sum_{m\neq n} |m\rangle \sum_{k\neq n} \frac{\langle m|\partial_\nu H|k\rangle\langle k|\partial_\mu H|n\rangle}{(E_n - E_m)(E_n - E_k)} - \sum_{m\neq n} |m\rangle \frac{\langle n|\partial_\nu H|n\rangle\langle m|\partial_\mu H|n\rangle}{(E_n - E_m)^2}.\end{aligned}$$

The calculation could proceed further order by order, but we will stop at the second order; very few practical problems are left which worths the effort and complexity of higher order perturbative calculations.

Let's discuss some physical pictures that can be seen from the above results. The power series of energies and states are

$$\begin{aligned}E_n(x^\mu) &= E_n + \sum_\nu \partial_\nu E_n x^\nu + \frac{1}{2}\sum_{\mu,\nu} \partial_\mu\partial_\nu E_n x^\mu x^\nu + \dots \\ |n(x^\mu)\rangle &= |n\rangle + \sum_\nu |\partial_\nu n\rangle x^\nu + \frac{1}{2}\sum_{\mu,\nu} |\partial_\mu\partial_\nu n\rangle x^\mu x^\nu + \dots\end{aligned}$$

The convergence range would depend on the magnitudes of the derivatives, and thus, according the above results, the magnitude of the "perturbation" $\langle m|\partial_\mu H|n\rangle$ comparing to the magnitude of the "energy gap" $E_n - E_m$. Therefore, non-degeneracy is indeed a good assumption. We may define the perturbation strength Λ to be the average of $|\langle m|\partial_\mu H|n\rangle|$, then the states $|m\rangle$ with $E_n - E_m \gg \Lambda$ will have negligible contribution to the correction of $|n\rangle$. Therefore, it is good to think that a perturbation of strength Λ introduces interactions between, and mix, only states whose energy difference is smaller or comparable to Λ. As a result, the physics laws at different energy scales can be separated.

6.2 Effective Hamiltonian

When some of the energy levels are nearly degenerate or even exactly degenerate, one should expect a bad behavior of the perturbative expansion. Let's take a look at the exactly degenerate case. Without loss of generality, assume E_n are all the same for $1 \leq n \leq D$. In this case, the first D basis states are no longer well defined up to a phase; instead, they are together defined up to a $D \times D$ unitary matrix U. Therefore, we have to modify, for example, the first order perturbative equation

$$(\partial_\nu E_n - \partial_\nu H)U|n\rangle + (E_n - H)U|\partial_\nu n\rangle = 0, \quad n = 1, \ldots, D.$$

Project the above to $\langle m|,\ m = 1, \ldots, D$, we get

$$\partial_\nu E_n \langle m|U|n\rangle = \langle m|\partial_\nu H U|n\rangle,$$

which is nothing but the eigenvalue problem of $\partial_\nu H$ restricted in the $D \times D$ degenerate subspace. However, if we could easily solve the eigenvalue problem (exact diagonalization), we would not even attempt the perturbative approach.

Nonetheless, we may try the second best. Suppose we do have the power to do the exact diagonalization within the degenerate subspace. We are thus satisfied if we can block-diagonalize the Hamiltonian with respect to the degenerate subspaces. In better terms, we are going to derive the effective Hamiltonian in a subspace. The subspace does not necessarily have (nearly) degenerate energy; as long as the energy separation between this subspace and the remainder is large enough, we have a good effective theory.

Consider the Hamiltonian $H(x^\mu)$ which is diagonal at $x^\mu = 0$,

$$H|n\rangle = E_n|n\rangle.$$

Assume that $|E_n - E_m| \gg 0$ for $1 \leq n \leq D$ and $m > D$. Define projection operators

$$P = \sum_{n=1}^{D} |n\rangle\langle n|, \quad Q = 1 - P = \sum_{m>D} |m\rangle\langle m|.$$

Note the properties of the projections

$$1 = P + Q,\ P^2 = P,\ Q^2 = Q,\ PQ = 0,\ QP = 0.$$

Define the block diagonal part of an operator A

$$A_{\mathrm{bD}} = PAP + QAQ,$$

as well the block off-diagonal part

$$A_{\mathrm{bO}} = A - A_{\mathrm{bD}} = PAQ + QAP.$$

Our goal is to introduce a unitary transformation $U(x^\mu) = \mathrm{e}^{\mathrm{i}S(x^\mu)}$ such that $U(x^\mu)H(x^\mu)U^\dagger(x^\mu)$ remains block diagonal as we turn on the perturbation, i.e., increase x^μ. First use the Hadamard formula,

$$U(x^\mu)H(x^\mu)U^\dagger(x^\mu) = \mathrm{e}^{[\mathrm{i}S(x^\mu),-]}H(x^\mu) = \sum_k \frac{1}{k!}[\mathrm{i}S(x^\mu),-]^k H(x^\mu).$$

We want the block off-diagonal entries to be zero:

$$\begin{aligned} 0 &= \left(\sum_k \frac{1}{k!}[\mathrm{i}S(x^\mu),-]^k H(x^\mu)\right)_{\mathrm{bO}} \\ &= \left(\sum_k \frac{1}{k!}[\mathrm{i}S_{\mathrm{bD}}(x^\mu) + \mathrm{i}S_{\mathrm{bO}}(x^\mu),-]^k H(x^\mu)\right)_{\mathrm{bO}} \end{aligned}$$

The above is a function equation for the block off-diagonal entries. We have more variables $S_{\mathrm{bD}}(x^\mu)$ and $S_{\mathrm{bO}}(x^\mu)$ than equations. Intuitively, the block-diagonal part of S is rotating the states in the subspaces. This work should be left after the effective Hamiltonian is found. Thus, we may set $S_{\mathrm{bD}}(x^\mu) \equiv 0$. The equation is simplified with block off-diagonal $S(x^\mu) = S_{\mathrm{bO}}(x^\mu)$ but still solvable. It is easy to check that the product of two block off-diagonal operators is block diagonal, and the product of a block diagonal operator and a block off-diagonal operator is block off-diagonal. Therefore,

$$\begin{aligned} 0 &= \left(\sum_k \frac{1}{k!}[\mathrm{i}S(x^\mu),-]^k H(x^\mu)\right)_{\mathrm{bO}} \\ &= \sum_k \frac{1}{2k!}[\mathrm{i}S_{\mathrm{bO}}(x^\mu),-]^{2k} H_{\mathrm{bO}}(x^\mu) \\ &+ \sum_k \frac{1}{(2k+1)!}[\mathrm{i}S_{\mathrm{bO}}(x^\mu),-]^{2k+1} H_{\mathrm{bD}}(x^\mu). \end{aligned}$$

Or more compactly

$$\begin{aligned} \cos[S_{\mathrm{bO}}(x^\mu),-]H_{\mathrm{bO}}(x^\mu) + \mathrm{i}\sin[S_{\mathrm{bO}}(x^\mu),-]H_{\mathrm{bD}}(x^\mu) = 0, \\ H_{\mathrm{bO}}(x^\mu) + \mathrm{i}\tan[S(x^\mu),-]H_{\mathrm{bD}}(x^\mu) = 0. \end{aligned}$$

We will work out the first and second orders. Note that H is diagonal, thus $H_{\mathrm{bD}} = H,\ H_{\mathrm{bO}} = 0$. Setting $x^\mu = 0$ in the first derivative leads to

$$\partial_\nu H_{\mathrm{bO}} + \mathrm{i}[\partial_\nu S, H] = 0.$$

Check the matrix elements

$$\langle m|\partial_\nu H_{\mathrm{bO}}|n\rangle + \mathrm{i}(E_n - E_m)\langle m|\partial_\nu S|n\rangle = 0.$$

Thus,

$$\mathrm{i}\partial_\nu S = \sum_{m,n} |m\rangle \frac{\langle m|\partial_\nu H_{\mathrm{bO}}|n\rangle}{E_m - E_n}\langle n|.$$

The block off-diagonal operator automatically enforces the condition that m, n belongs to different subspaces.

The second order equation is

$$\partial_\mu\partial_\nu H_{\mathrm{bO}} + \mathrm{i}[\partial_\mu\partial_\nu S, H] + \mathrm{i}[\partial_\mu S, \partial_\nu H_{\mathrm{bD}}] + \mathrm{i}[\partial_\nu S, \partial_\mu H_{\mathrm{bD}}] = 0.$$

Again, check the matrix elements

$$\begin{aligned}
&\langle m|\partial_\mu\partial_\nu H_{\mathrm{bO}}|n\rangle + \mathrm{i}(E_n - E_m)\langle m|\partial_\mu\partial_\nu S|n\rangle \\
&= -\mathrm{i}\langle m|[\partial_\mu S, \partial_\nu H_{\mathrm{bD}}]|n\rangle - \mathrm{i}\langle m|[\partial_\nu S, \partial_\mu H_{\mathrm{bD}}]|n\rangle \\
&= \sum_k \frac{\langle m|\partial_\mu H_{\mathrm{bO}}|k\rangle\langle k|\partial_\nu H_{\mathrm{bD}}|n\rangle}{E_k - E_m} - \frac{\langle m|\partial_\mu H_{\mathrm{bD}}|k\rangle\langle k|\partial_\nu H_{\mathrm{bO}}|n\rangle}{E_n - E_k} \\
&+ \sum_k \frac{\langle m|\partial_\nu H_{\mathrm{bO}}|k\rangle\langle k|\partial_\mu H_{\mathrm{bD}}|n\rangle}{E_k - E_m} - \frac{\langle m|\partial_\nu H_{\mathrm{bD}}|k\rangle\langle k|\partial_\mu H_{\mathrm{bO}}|n\rangle}{E_n - E_k},
\end{aligned}$$

from which $\partial_\mu\partial_\nu S$ can be determined. The expression is becoming too long; also, the contribution of $\partial_\mu\partial_\nu S$ to the Hamiltonian up to the second order is through $[\partial_\mu\partial_\nu S, H]$ which is block off-diagonal, so we do not need it for the second order effective Hamiltonian. $\partial_\mu\partial_\nu S$ does contribute to the the state correction, though.

Let's conclude this section by writing down the effective Hamiltonian to the

second order.

$$
\begin{aligned}
&S(x^\mu) = \sum_\mu x^\mu \partial_\mu S + \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu \partial_\mu\partial_\nu S + \dots,\\
&H_{\text{eff}}(x^\mu) := P\mathrm{e}^{[\mathrm{i}S(x^\mu),-]}H(x^\mu)P\\
&= PHP + \sum_\mu x^\mu P\partial_\mu HP + \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P\partial_\mu\partial_\nu HP\\
&+ \sum_\mu x^\mu P[\mathrm{i}\partial_\mu S, H]P\\
&+ \sum_{\mu\nu} x^\mu x^\nu P[\mathrm{i}\partial_\mu S, \partial_\nu H]P + \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P[\mathrm{i}\partial_\mu\partial_\nu S, H]P\\
&+ \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P[\mathrm{i}\partial_\mu S, [\mathrm{i}\partial_\nu S, H]]P + \dots\\
&= PHP + \sum_\mu x^\mu P\partial_\mu HP + \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P\partial_\mu\partial_\nu HP\\
&+ \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P[\mathrm{i}\partial_\mu S, \partial_\nu H]P + \dots\\
&= PHP + \sum_\mu x^\mu P\partial_\mu HP + \frac{1}{2}\sum_{\mu\nu} x^\mu x^\nu P\partial_\mu\partial_\nu HP\\
&+ \frac{1}{2}\sum_{\substack{\mu\nu\\ 1\le m\le D\\ 1\le n\le D\\ k>D}} x^\mu x^\nu |m\rangle \left(\frac{\langle m|\partial_\mu H|k\rangle\langle k|\partial_\nu H|n\rangle}{E_m - E_k} + \frac{\langle m|\partial_\nu H|k\rangle\langle k|\partial_\mu H|n\rangle}{E_n - E_k}\right)\langle n|\\
&+ \dots.
\end{aligned}
$$

You may check that when $D = 1$, the one-dimensional effective Hamiltonian agrees with our previous results on non-degenerate perturbation theory.

6.3 Scattering theory

In this section we introduce some basic formulism of quantum scattering theory. Scattering theory is extremely useful in practice: we get to know a new object by looking at how other things are scattered by this object; indeed, our eyes and ears are just detectors working this way.

In the non-relativistic quantum setting, the scatterer we want to study is represented by a potential V, usually with finite support (non-zero in a finite range). A beam of known particles are thrown to the potential, and we consider a total Hamiltonian

$$H + V, \quad H = \frac{\hat{p}^2}{2m}.$$

A practical scattering process is dynamical, and involves wave packets of particles which are finite in both space and time. However, due to the linearity of quantum mechanics, it is much more clear to study the basis eigenstates, which are steady. Consider that we launch an infinite plane wave to the scatterer, and allow a long enough evolution until the state becomes steady, i.e., an eigenstate. For this to happen, it is necessary that V is independent of time, or in other words, energy is preserved and the scattering is elastic. The states with a different energy than the incoming plane wave would interfere destructively; some other perturbations could also help these "non-resonant" states to dissipate. The resulting steady state should be an eigenstate with the same energy as the incoming plane wave. Mathematically, we want to find the eigenstate $|\psi\rangle$

$$(H + V)|\psi\rangle = E|\psi\rangle,$$

with the "boundary condition" that as $V \to 0$, $|\psi\rangle$ approaches the plane wave state $|\psi\rangle \to |p\rangle$, $E = p^2/2m$. To fit such "boundary condition", we may rewrite

$$V|\psi\rangle = (E - H)|\psi\rangle.$$

We know the "general solutions" to the right hand side

$$0 = (E - H)|\psi\rangle,$$

which are just the plane wave eigenstates $|p\rangle$, and we need some "special solution" to produce the left hand side.

It will be nice if we can somehow "invert" the operator $(E - H)$. Consider a more general form of linear equation

$$Ax = y.$$

If there is a left inverse L of A, ($LA = 1$, but not necessarily $AL = 1$), then the solution must be unique if exists, since by multiplying L we have $LAx = x = Ly$. However, it is possible that $x = Ly$ is not even a solution. On the other hand, if there is a right inverse G of A, ($AG = 1$ but not necessarily $GA = 1$), we do have a special solution $x = Gy$ which satisfies $Ax = AGy = y$. For a linear operator A that we know many general solutions to $Ax = 0$ exist, which can be combined with a special solution to $Ax = y$ to produce other solutions, clearly we can at most count on the right inverse. This is the idea behind the Green's function method.

A Green's function is just a right inverse.

The right inverse is not unique in general, and may account for different initial or boundary conditions. The right inverse G of $E - H$, in the position basis, is the Green's function $G(x, y) = \langle x|G|y\rangle$ satisfying

$$\delta(x - y) = \langle x|y\rangle = \langle x|(E - H)G|y\rangle = (E + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})G(x, y),$$

Similar to the delta function, the Green's function should also be considered as a generalized function, i.e., defined by its action via the integral against test wavefunctions. This point of view also explains why a singular operator $E-H$ can be inverted: the states with $E-H$ being zero occupies only a zero measure comparing to all the states (two points comparing to a line, a circle comparing to a plane, a sphere comparing to a bulk, depending on dimensions). Surely for the majority of the states we just take $\frac{1}{E-H}$; the tricky thing is how to deal with the singular parts.

Again, similar to how one can approximate the delta function, the Green's function can be approximated by some sequence of functions with the limit taking outside the integral. A good prescription here is to make the energy slightly complex so that it is no longer singular,

$$G_\pm := \frac{1}{E \pm \mathrm{i}\epsilon - H}.$$

Here, $\epsilon > 0$ is a small positive number. The sign will affect the boundary conditions as we will see later. The limit $\epsilon \to 0$ is to be taken at the end of the calculation. We arrive at the Lippmann-Schwinger equation

$$|\psi\rangle_\pm = |p\rangle + G_\pm V|\psi\rangle_\pm = |p\rangle + \frac{1}{E \pm \mathrm{i}\epsilon - H} V|\psi\rangle_\pm.$$

In the Lippmann-Schwinger equation we like to set $E = p^2/2m$. Since the direction of p matters as the boundary condition in a scattering problem, for convenience we introduce the the positive wavenumber $k > 0$, $\hbar k = |p| = \sqrt{2mE}$ and separate the sign of $p = \pm\hbar k$ out.

Let's work out the one-dimensional Green's function explicitly

$$\begin{aligned}\langle x|G_+|y\rangle &= \int \mathrm{d}q \, \langle x|q\rangle\langle q|\frac{1}{E + \mathrm{i}\epsilon - H}|y\rangle \\ &= \frac{m}{\pi\hbar}\int \mathrm{d}q \, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}q(x-y)}}{\hbar^2k^2 + \mathrm{i}\epsilon - q^2}.\end{aligned}$$

For a simpler notation, ϵ multiplied by a positive constant is still denoted by ϵ; it is to be taken to zero in the end anyway. The integral is computed by picking a proper contour in the complex plane of q. For $x - y > 0$, we should pick a half circle in the upper half plane to ensure convergence. The integrand has two poles at

$$q = \pm\sqrt{\hbar^2k^2 + \mathrm{i}\epsilon} \approx \pm(\hbar k + \mathrm{i}\epsilon),$$

The pole with a positive sign before k, $q = \hbar k + \mathrm{i}\epsilon$ is enclosed in the upper half plane contour. The contour is anti-clockwise. The residue is $-\frac{\mathrm{e}^{\mathrm{i}k(x-y)-\epsilon}}{2\hbar k+\mathrm{i}\epsilon}$ which can be seen from the expansion

$$\frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}q(x-y)}}{\hbar^2k^2 + \mathrm{i}\epsilon - q^2} = \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}q(x-y)}}{2\hbar k + \mathrm{i}\epsilon}\left(\frac{1}{q + \hbar k + \mathrm{i}\epsilon} - \frac{1}{q - \hbar k - \mathrm{i}\epsilon}\right),$$

therefore,

$$\int \mathrm{d}q \, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}q(x-y)}}{\hbar^2 k^2 + \mathrm{i}\epsilon - q^2} = -2\pi\mathrm{i}\frac{\mathrm{e}^{\mathrm{i}k(x-y)-\epsilon}}{2\hbar k + \mathrm{i}\epsilon} \to -\pi\mathrm{i}\frac{\mathrm{e}^{\mathrm{i}k(x-y)}}{\hbar k},$$

for $x - y > 0$. Similarly we can compute the case $x - y < 0$, where the contour should be the lower half plane, clockwise. The sign from the orientation of the contour cancels the sign difference between the residue of the two poles, thus only the sign difference in the exponent remains,

$$\int \mathrm{d}q \, \frac{\mathrm{e}^{\frac{\mathrm{i}}{\hbar}q(x-y)}}{\hbar^2 k^2 + \mathrm{i}\epsilon - q^2} = -2\pi\mathrm{i}\frac{\mathrm{e}^{-\mathrm{i}k(x-y)-\epsilon}}{2\hbar k + \mathrm{i}\epsilon} \to -\pi\mathrm{i}\frac{\mathrm{e}^{-\mathrm{i}k(x-y)}}{\hbar k},$$

for $x-y < 0$. For G_-, the sign before k for the two poles are switched comparing to G_+. Concluding all cases,

$$\langle x|G_\pm|y\rangle = \frac{2m}{\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}k|x-y|}}{\pm 2\mathrm{i}k}.$$

Problem 6.3.1. 1. As a consistent check of the above solution, use the step function $\theta(x)$ with

$$\frac{\partial\theta(x)}{\partial x} = \delta(x), \quad \frac{\partial|x|}{\partial x} = \theta(x) - \theta(-x),$$

and compute the second derivative of $\mathrm{e}^{\pm\mathrm{i}k|x|}$.

2. Think about why

$$\langle x|G_\pm(E-H)|y\rangle = (E + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2})\langle x|G_\pm|y\rangle = \delta(x-y),$$

but $G_\pm$ is not a left inverse to $E - H$.

We now have

$$\langle x|\psi\rangle_\pm = \langle x|p\rangle + \int \mathrm{d}y \, \frac{m}{\mathrm{i}\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}k|x-y|}}{\pm k}\langle y|V|\psi\rangle_\pm.$$

Instead of solving this integral equation, we are more interested in the asymptotic behavior as $x \to \infty$, as in practice we usually measure the scattered wave at far away from the scatterer. At $x \to +\infty$, $|x-y| = x - y$,

$$\langle x|\psi\rangle_\pm = \langle x|p\rangle + \mathrm{e}^{\pm\mathrm{i}kx}\int \mathrm{d}y \, \frac{m}{\mathrm{i}\hbar^2}\frac{\mathrm{e}^{\mp\mathrm{i}ky}}{\pm k}\langle y|V|\psi\rangle_\pm.$$

At $x \to -\infty$, $|x-y| = -x + y$,

$$\langle x|\psi\rangle_\pm = \langle x|p\rangle + \mathrm{e}^{\mp\mathrm{i}kx}\int \mathrm{d}y \, \frac{m}{\mathrm{i}\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}ky}}{\pm k}\langle y|V|\psi\rangle_\pm.$$

In fact x does not need to be too large; as long as x is outside the support of V, the above asymptotic behaviors are exact. We see that the positive solution describes plane waves going away from the scatterer while the negative solution describes plane waves going to the scatterer, which is the time-reversal of the positive solution. We thus focus on the positive solution. Without loss of generality, let's take $p = \hbar k$, i.e., incoming plane wave from the left. One can see that

$$\langle x|\psi\rangle_L \sim \begin{cases} a\,\mathrm{e}^{\mathrm{i}kx}, & x \to +\infty, \\ \mathrm{e}^{\mathrm{i}kx} + b\,\mathrm{e}^{-\mathrm{i}kx}, & x \to -\infty. \end{cases}$$

Where a, b are coefficients depending on both k and the scatter potential V. Physically, a is the transmission amplitude and b is the reflection amplitude. We have the relation

$$1 = |a|^2 + |b|^2,$$

as the result of probability conservation. To prove it, we may use the *current* corresponding to probability conservation. For a more general application, let's consider the problem in arbitrary dimensions. Given a time dependant state $|\Psi(t)\rangle = U(t)|\Psi\rangle$ satisfying the Schrodinger equation,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle = \left(\frac{\hat{\boldsymbol{p}}^2}{2m} + V\right)|\Psi(t)\rangle.$$

In the position basis

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\langle \boldsymbol{r}|\Psi(t)\rangle = \left(-\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r})\right)\langle \boldsymbol{r}|\Psi(t)\rangle.$$

The total probability is conserved since the evolution $U(t)$ is unitary

$$\langle\Psi(t)|\Psi(t)\rangle = \langle\Psi|\Psi\rangle.$$

Now consider a closed manifold M with boundary ∂M. The probability of finding the particle in M at time t is

$$\int_M \mathrm{d}\boldsymbol{r}\,\langle\Psi(t)|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\Psi(t)\rangle.$$

Use the shorthand notation $\Psi := \langle \boldsymbol{r}|\Psi(t)\rangle$, and calculate the time derivative while substituting in the Schrodinger equation

$$\begin{aligned} -\frac{\partial}{\partial t}\int_M \mathrm{d}\boldsymbol{r}\,\Psi^*\Psi &= \int_M \mathrm{d}\boldsymbol{r}\,\Psi^*\frac{\mathrm{i}}{\hbar}\left(-\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r})\right)\Psi - \Psi\frac{\mathrm{i}}{\hbar}\left(-\frac{\hbar^2\nabla^2}{2m} + V(\boldsymbol{r})\right)\Psi^* \\ &= \int_M \mathrm{d}\boldsymbol{r}\,\frac{-\mathrm{i}\hbar}{2m}\left(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right) \\ &= \int_M \mathrm{d}\boldsymbol{r}\,\frac{-\mathrm{i}\hbar}{2m}\nabla\cdot\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) \\ &= \int_{\partial M} \mathrm{d}\boldsymbol{S}\cdot\frac{-\mathrm{i}\hbar}{2m}(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) \end{aligned}$$

Thus we can associate the probability current to Ψ,

$$\boldsymbol{j}_\Psi(\boldsymbol{r},t)=\frac{-\mathrm{i}\hbar}{2m}\bigg(\langle\Psi(t)|\boldsymbol{r}\rangle\nabla\langle\boldsymbol{r}|\Psi(t)\rangle-\langle\boldsymbol{r}|\Psi(t)\rangle\nabla\langle\Psi(t)|\boldsymbol{r}\rangle\bigg).$$

In particular, for a steady eigenstate,

$$\int_{\partial M}\mathrm{d}\boldsymbol{S}\cdot\boldsymbol{j}=0,$$

which means in one dimension that j is a constant with respect to position. Then, for the asymptotic wavefunctions, at $x\to+\infty$,

$$\langle x|\psi\rangle_L\sim a\,\mathrm{e}^{\mathrm{i}kx},$$

we have

$$j(x)\sim\frac{-\mathrm{i}\hbar}{2m}\left(a^*\mathrm{e}^{-\mathrm{i}kx}\frac{\partial}{\partial x}a\mathrm{e}^{\mathrm{i}kx}-a\mathrm{e}^{\mathrm{i}kx}\frac{\partial}{\partial x}a^*\mathrm{e}^{-\mathrm{i}kx}\right)=\frac{\hbar k}{m}|a|^2.$$

At $x\to-\infty$,

$$\langle x|\psi\rangle_L\sim\mathrm{e}^{\mathrm{i}kx}+b\,\mathrm{e}^{-\mathrm{i}kx},$$

we have

$$\begin{aligned}j(x)\sim\frac{-\mathrm{i}\hbar}{2m}\Big((\mathrm{e}^{-\mathrm{i}kx}+b^*\,\mathrm{e}^{\mathrm{i}kx})\frac{\partial}{\partial x}(\mathrm{e}^{\mathrm{i}kx}+b\,\mathrm{e}^{-\mathrm{i}kx})\\-(\mathrm{e}^{\mathrm{i}kx}+b\,\mathrm{e}^{-\mathrm{i}kx})\frac{\partial}{\partial x}(\mathrm{e}^{-\mathrm{i}kx}+b^*\,\mathrm{e}^{\mathrm{i}kx})\Big)=\frac{\hbar k}{m}(1-|b|^2).\end{aligned}$$

Therefore, we indeed obtain $1-|b|^2=|a|^2$. For the case $p=-\hbar k$, i.e., incoming plane from the right instead of the left, we may exploit the time-reversal symmetry of the Hamiltonian, which means that $\langle x|\psi\rangle_L^*$ is also a solution to the Schrodinger equation. We can then combine $\langle x|\psi\rangle_L^*$ with $\langle x|\psi\rangle_L$ to obtain the correct asymptotic form, which turns out to be

$$\langle x|\psi\rangle_R=\frac{1}{a^*}\bigg(\langle x|\psi\rangle_L^*-b^*\langle x|\psi\rangle_L\bigg)=\begin{cases}\mathrm{e}^{-\mathrm{i}kx}-b^*\frac{a}{a^*}\mathrm{e}^{\mathrm{i}kx}, & x\to+\infty,\\ \frac{1-|b|^2}{a^*}\mathrm{e}^{-\mathrm{i}kx}=a\,\mathrm{e}^{-\mathrm{i}kx}, & x\to-\infty.\end{cases}$$

We can see that the transmission amplitude a remains the same, while the reflection amplitude $b^*\frac{a}{a^*}$ differs from b by a phase factor.

The scattering theory in two dimensions is less straightforward. The Green's function is given by a Hankel function instead of some combinations of elementary functions as in one and three dimensions.

Problem 6.3.2. Compute

$$G_\pm(\boldsymbol{r},\boldsymbol{r}')=\langle\boldsymbol{r}|\frac{1}{E\pm\mathrm{i}\epsilon-H}|\boldsymbol{r}'\rangle,$$

in two and three dimensions explicitly by inserting the momentum resolution of identity, transforming into the polar coordinates, and then using the method of contour integral. In two dimensions, the Mehler's Bessel function formula can be useful

$$J_0(x) = \frac{2}{\pi}\int_0^\infty \sin(x\cosh t)\mathrm{d}t, \quad Y_0(x) = -\frac{2}{\pi}\int_0^\infty \cos(x\cosh t)\mathrm{d}t.$$

Also

$$\int_0^{2\pi} \mathrm{e}^{\mathrm{i}x\cos\theta}\mathrm{d}\theta = 2\pi J_0(x),$$

and the Hankel functions are

$$H_\alpha^+(x) = J_\alpha(x) + \mathrm{i}Y_\alpha(x), \quad H_\alpha^-(x) = J_\alpha(x) - \mathrm{i}Y_\alpha(x).$$

Up to a normalization factor, $G_\pm$ is given by $H_0^\pm$.

We then discuss some important notions in the scattering theory in three dimensions. Firstly, the Green's function in three dimensions is

$$G_\pm(\boldsymbol{r},\boldsymbol{r}') = \langle \boldsymbol{r}|\frac{1}{E\pm\mathrm{i}\epsilon - H}|\boldsymbol{r}'\rangle = -\frac{2m}{\hbar^2}\frac{\mathrm{e}^{\pm\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|},$$

where $\hbar k = \sqrt{2mE}$.

Again, we are interested in the positive solution at far away from the scatterer,

$$\begin{aligned}\langle \boldsymbol{r}|\psi\rangle &= \langle \boldsymbol{r}|\boldsymbol{p}\rangle + \int \mathrm{d}\boldsymbol{r}'\, G_+(\boldsymbol{r},\boldsymbol{r}')\langle \boldsymbol{r}'|V|\psi\rangle \\ &= \langle \boldsymbol{r}|\boldsymbol{p}\rangle - \frac{2m}{4\pi\hbar^2}\int \mathrm{d}\boldsymbol{r}'\,\frac{\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|}}{|\boldsymbol{r}-\boldsymbol{r}'|}\langle \boldsymbol{r}'|V|\psi\rangle,\end{aligned}$$

where $\boldsymbol{p} = \hbar\boldsymbol{k}$, $k = |\boldsymbol{k}|$. At $r := |\boldsymbol{r}| \to \infty$, we have

$$|\boldsymbol{r}-\boldsymbol{r}'| = \sqrt{(\boldsymbol{r}-\boldsymbol{r}')\cdot(\boldsymbol{r}-\boldsymbol{r}')} \sim r - \frac{\boldsymbol{r}}{r}\cdot\boldsymbol{r}'.$$

Denote the unit vector by $\mathbf{n}_r := \boldsymbol{r}/r$, then

$$\mathrm{e}^{\mathrm{i}k|\boldsymbol{r}-\boldsymbol{r}'|} \sim \mathrm{e}^{\mathrm{i}kr}\mathrm{e}^{-\mathrm{i}k\mathbf{n}_r\cdot\boldsymbol{r}'}.$$

Further denoting the radial wave vector by $\boldsymbol{k}_r := k\mathbf{n}_r$, the asymptotic wavefunction is

$$\begin{aligned}\langle \boldsymbol{r}|\psi\rangle &\sim \langle \boldsymbol{r}|\boldsymbol{p}\rangle - \frac{\mathrm{e}^{\mathrm{i}kr}}{r}\frac{2m}{4\pi\hbar^2}\int \mathrm{d}\boldsymbol{r}'\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}_r\cdot\boldsymbol{r}'}\langle \boldsymbol{r}'|V|\psi\rangle \\ &\sim \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f(\boldsymbol{k}_r,\boldsymbol{k})\frac{\mathrm{e}^{\mathrm{i}kr}}{r}.\end{aligned}$$

Here, the physical meaning of $f(\boldsymbol{k}_r, \boldsymbol{k})$ is the amplitude for particles to be scattered into unit solid angle along the direction $\mathbf{n}_r$, similar to the transmission and reflection amplitude in the one-dimensional case. Moreover, $|f(\boldsymbol{k}_r, \boldsymbol{k})|^2$ can be identified as the *differential cross section*.

To explain the notion of cross section, consider that a plane wave of particles are thrown to a scatterer. When detecting from far away on the other side, since the density of the scattered particles decays with $1/r^2$, it is expected to see a plane wave with a "hole" around the scatterer. The area of the "hole" reflects the power of the scatterer and the *total cross section* σ is just defined as the area of such "hole". Then, pick a small area $\mathrm{d}\sigma$ in this "hole". Classically one may track the particle trajectories to find to which direction $\mathbf{n}_r$ the incident particles in $\mathrm{d}\sigma$ are scattered. Quantum mechanically, it is also possible to establish a similar picture for a steady state by looking at the probability current (or particle flux) vector $\boldsymbol{j}$. Suppose that the incident flux is j_i and the scattering flux at $\boldsymbol{r}$ along the radial direction is j_r. Then, $j_i \mathrm{d}\sigma$ is incident particle number per unit time; $j_r r^2 \mathrm{d}\Omega$ is the scattered particle number per unit time, where $\mathrm{d}\Omega$ is the solid angle. The two quantities should be equal. The differential cross section is defined as $\mathrm{d}\sigma/\mathrm{d}\Omega$, namely, the area scattered away into unit solid angle.

Since we are considering an elastic scattering process, the incident wave and scattered wave share the same magnitude of wave vector, or the same "velocity". We can thus even avoid the calculation of flux and simply check the density. It is enough to consider the relative density. With the density of the incident wave set to 1, the relative density of the scattered wave at $\boldsymbol{r}$ is $|f(\boldsymbol{k}_r, \boldsymbol{k})/r|^2$. Therefore,

$$1 \cdot \mathrm{d}\sigma = |f(\boldsymbol{k}_r, \boldsymbol{k})/r|^2 r^2 \mathrm{d}\Omega \,.$$

Indeed we have

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\boldsymbol{k}_r, \boldsymbol{k})|^2.$$

Note that the total density or flux definitely involves the interference between the incident wave and the scattered wave. $f(\boldsymbol{k}_r, \boldsymbol{k})$ is only an indirect observable that can be extracted by proper manipulation on the measurement results of density or flux.

Problem 6.3.3. To get more intuition about three dimensional scattering, compute the probability current $\boldsymbol{j}(\boldsymbol{r})$ associated to the wavefunction

$$\langle \boldsymbol{r}|\psi\rangle = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f_k(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r},$$

where we take the convention that $\boldsymbol{k} = k\mathbf{n}_z$ points to the $+z$ direction, and $f(\boldsymbol{k}_r, \boldsymbol{k}) = f(k\mathbf{n}_r, k\mathbf{n}_z) = f_k(\mathbf{n}_r) = f_k(\theta, \phi)$.

1. Show that the gradient of an arbitrary function $F(r, \theta, \phi)$ in three dimensional polar coordinates reads

$$\nabla F = \frac{\partial F}{\partial r}\mathbf{n}_r + \frac{1}{r}\frac{\partial F}{\partial \theta}\mathbf{n}_\theta + \frac{1}{r\sin\theta}\frac{\partial F}{\partial \phi}\mathbf{n}_\phi,$$

where $\mathbf{n}_r, \mathbf{n}_\theta, \mathbf{n}_\phi$ denotes the unit vectors pointing to the directions along which r, θ, ϕ increase, respectively. Also the current $\boldsymbol{j}(\boldsymbol{r})$ may be represented more compactly by taking the imaginary part $\Im$

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{\hbar}{m}\Im\left(\langle\psi|\boldsymbol{r}\rangle\nabla\langle\boldsymbol{r}|\psi\rangle\right).$$

2. Compute

$$\begin{aligned}\nabla\langle\boldsymbol{r}|\psi\rangle = \mathrm{i}\boldsymbol{k}\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} + f_k\left(\mathrm{i}k\frac{\mathrm{e}^{\mathrm{i}kr}}{r} - \frac{\mathrm{e}^{\mathrm{i}kr}}{r^2}\right)\mathbf{n}_r \\ + \frac{\mathrm{e}^{\mathrm{i}kr}}{r^2}\left(\frac{\partial f_k}{\partial\theta}\mathbf{n}_\theta + \frac{1}{\sin\theta}\frac{\partial f_k}{\partial\phi}\mathbf{n}_\phi\right).\end{aligned}$$

3. Show that the current may be separated into three parts: the incident part

$$\boldsymbol{j}_{\text{incident}} = \frac{\hbar}{m}\boldsymbol{k},$$

the interfering part

$$\boldsymbol{j}_{\text{interfering}} \sim \mathrm{e}^{\mathrm{i}kr(1-\cos\theta)},$$

and the scattered part

$$\boldsymbol{j}_{\text{scattered}} = \frac{\hbar k}{m}\frac{|f_k|^2}{r^2}\mathbf{n}_r + O\left(\frac{1}{r^3}\right)\mathbf{n}_\theta + O\left(\frac{1}{r^3}\right)\mathbf{n}_\phi.$$

Try to explain why for large enough r, we can think

$$\boldsymbol{j} \approx \frac{\hbar k}{m}\left(\mathbf{n}_z + \frac{|f_k|^2}{r^2}\mathbf{n}_r\right).$$

It worths mentioning the special case when $V(\boldsymbol{r}) = V(r)$ is rotationally invariant. Clearly the free Hamiltonian $H = \frac{\boldsymbol{p}^2}{2m}$ is also rotationally invariant. It is then great to solve the problem in the (orbital) angular momentum basis. When dealing with an incident plane wave, this approach is referred to as the *partial wave* method. As some complicated mathematics regarding spherical functions are involved, we will not elaborate on the details. However, due to the conservation of angular momentum, there is an important result by considering an incoming wave and an outgoing wave with the same angular momentum. The asymptotic wavefunction is

$$\langle\boldsymbol{r}|\psi\rangle \sim \big(\frac{\mathrm{e}^{-\mathrm{i}kr}}{r} + f_l^m\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\big)Y_l^m(\theta,\phi).$$

Conservation of probability tells us that f_l^m has to be a phase factor $|f_l^m| = 1$, known as the *phase shift*.

Problem 6.3.4. Verify $|f_l^m| = 1$ for the state

$$\langle \boldsymbol{r}|\psi\rangle = \big(\frac{\mathrm{e}^{-\mathrm{i}kr}}{r} + f_l^m \frac{\mathrm{e}^{\mathrm{i}kr}}{r}\big) Y_l^m(\theta,\phi),$$

by considering the total current going through a sphere S^2

$$\int_{S^2} \boldsymbol{j} \cdot \mathrm{d}\boldsymbol{S} = 0.$$