Quantum Physics Exercise Class I

Yu Su

Hefei National Research Center for Physical Sciences at the Microscale, University of Science and Technology of China

Sep 10, 2023

Hilbert space

- A linear space $\mathcal{H}$ composed of $|\psi\rangle$
- Dual correspondence: $c|\psi\rangle \ \Leftrightarrow\ c^*\langle\psi|$
- Inner product: $\mathcal{H}\times\mathcal{H}\to\mathbb{C}$, or $\langle\psi|\varphi\rangle\in\mathbb{C}$, satisfying $\langle\psi|\varphi\rangle^* = \langle\varphi|\psi\rangle$

Note:

- The dimension of Hilbert space is determined by the physical requirements
- Proof of Cauchy–Schwarz inequality: Consider a vector

$$|\alpha\rangle \equiv |\psi\rangle + \lambda|\varphi\rangle \tag{1}$$

with $\lambda\in\mathbb{C}$. The inner product requires

$$\langle\alpha|\alpha\rangle = \langle\psi|\psi\rangle + \lambda\langle\psi|\varphi\rangle + \lambda^*\langle\varphi|\psi\rangle + |\lambda|^2\langle\varphi|\varphi\rangle \geq 0 \tag{2}$$

Let

$$\lambda = -\frac{\langle\varphi|\psi\rangle}{\langle\varphi|\varphi\rangle} \tag{3}$$

and we obtain the Cauchy–Schwarz inequality. The equality holds when

$$|\psi\rangle = -\lambda|\varphi\rangle \tag{4}$$

Hilbert space

Operator $\hat{A}$: $\mathcal{H} \to \mathcal{H}$

Note:

- Except for one special case, the operator is always a linear one, i.e.,

$$\hat{A}(c_1|\psi\rangle + c_2|\varphi\rangle) = c_1\hat{A}|\psi\rangle + c_2\hat{A}|\varphi\rangle \tag{5}$$

- Hermite conjugation ($\dagger$) of an operator $\hat{A}$ is defined via

$$\hat{A}|\psi\rangle \leftrightarrow \langle\psi|\hat{A}^\dagger \tag{6}$$

- Combination rule:

$$\langle\psi|(\hat{A}|\varphi\rangle) = (\langle\psi|\hat{A})|\varphi\rangle \equiv \langle\psi|\hat{A}|\varphi\rangle \tag{7}$$

- Hermite operator:

$$\hat{A} = \hat{A}^\dagger \tag{8}$$

  or in detail

$$(\langle\psi|\hat{A}|\varphi\rangle)^* = \langle\varphi|\hat{A}|\psi\rangle \tag{9}$$

- Outer product: $|\psi\rangle\langle\varphi|$ is an operator.

Eigenvalues and eigenvectors

The equation

$$\hat{A}|a_n\rangle = a_n|a_n\rangle \tag{10}$$

defines the eigenvalues $\{a_n\}$ and eigenvectors $\{|a_n\rangle\}$. Note:

- For an Hermitian, $a_n \in \mathbb{R}$ and the eigenvectors with different eigenvalues are orthogonal. The eigenvectors with the same eigenvalues span a subspace, therefore they can also be constructed orthogonally.
- In physical cases, any vector can be expanded by the eigenvectors in the same Hilbert space, namely

$$|\psi\rangle = \sum_n |a_n\rangle\langle a_n|\psi\rangle \tag{11}$$

or

$$1 = \sum_n |a_n\rangle\langle a_n| \quad \text{(Completeness)} \tag{12}$$

Here 1 should be explained as the unit operator in $\mathcal{H}$.

Representation

Given a set of complete eigenvectors, use them as basis and expand:

- vectors

$$|\psi\rangle = \sum_n |a_n\rangle\langle a_n|\psi\rangle \Longrightarrow \begin{bmatrix} \langle a_1|\psi\rangle \\ \langle a_2|\psi\rangle \\ \vdots \end{bmatrix} \tag{13}$$

$$\langle\psi| = \sum_n \langle\psi|a_n\rangle\langle a_n| \Longrightarrow \begin{bmatrix} \langle\psi|a_1\rangle & \langle\psi|a_2\rangle & \cdots \end{bmatrix} \tag{14}$$

- operators

$$\hat{A} = \sum_{mn} |a_m\rangle\langle a_m|\hat{A}|a_n\rangle\langle a_n| \equiv \sum_{mn} A_{mn}|a_m\rangle\langle a_n| \Longrightarrow \begin{bmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & A_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \equiv \mathbf{A} \tag{15}$$

In one representation, the vectors become $\dim\mathcal{H}^{\text{th}}$ dimensional arrays and operators become matrices $\in \mathbb{C}^{\dim\mathcal{H}\times\dim\mathcal{H}}$.

Representation

The unitary transformation links two different representation. Consider two basis $|a_n\rangle$ and $|b_n\rangle$. There exist two representations, being

$$|\psi\rangle = \sum_n |a_n\rangle\langle a_n|\psi\rangle = \sum_n |b_n\rangle\langle b_n|\psi\rangle \tag{16}$$

Hence we can define the unitary operator as

$$\hat{U} \equiv \sum_n |b_n\rangle\langle a_n| \tag{17}$$

with property

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1 \tag{18}$$

Then

$$\langle b_n|\psi\rangle = \sum_m \langle a_n|\hat{U}^\dagger|a_m\rangle\langle a_m|\psi\rangle = \langle a_n|\hat{U}^\dagger|\psi\rangle \tag{19}$$

With the same method, one can prove

$$\mathbf{A}' \equiv (\langle b_m|\hat{A}|b_n\rangle) = \mathbf{U}^\dagger\mathbf{A}\mathbf{U} \tag{20}$$

Representation

In order to solve the equation

$$\hat{B}|b\rangle = b|b\rangle \tag{21}$$

we firstly adopt one representation $|a_n\rangle$.Then we have

$$\sum_n \langle a_m|\hat{B}|a_n\rangle\langle a_n|b\rangle = b\langle a_m|b\rangle \tag{22}$$

or equivalently

$$\begin{bmatrix} B_{11} & B_{12} & \cdots \\ B_{21} & B_{22} & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix} = b \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix} \tag{23}$$

with $c_m \equiv \langle a_m|b\rangle$. Therefore, by solving the characteristic equation

$$\det(\mathbf{B} - \lambda\mathbf{I}) = 0 \tag{24}$$

one can obtain the eigenvalues and eigenvectors expressed by $|a_n\rangle$.

Some definitions

- Trace of an operator:

$$\operatorname{Tr}\hat{A} \equiv \sum_n \langle n|\hat{A}|n\rangle = \sum_n a_n \tag{25}$$

The definition holds only as the summation converges absolutely.

- Determinant:

$$\det\hat{A} \equiv \prod_n a_n \tag{26}$$

The definition also holds only as the product converges absolutely.

- Commutator and anticommutator:

$$[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A} \equiv [\hat{A},\hat{B}]_- \tag{27}$$

$$\{\hat{A},\hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A} \equiv [\hat{A},\hat{B}]_+ \tag{28}$$

And note that

$$[\hat{A},\hat{B}\hat{C}] = [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}] \tag{29}$$

Some definitions

- Function of an operator:

$$f(\hat{A}) \equiv \sum_{k=0}^{\infty} \frac{\hat{A}^k}{k!} f^{(k)}(0) \tag{30}$$

- Eigenvalues and eigenvectors:

$$f(\hat{A})|a_n\rangle = f(a_n)|a_n\rangle \tag{31}$$

- One important equality:

$$\det \hat{A} = e^{\mathrm{Tr} \ln \hat{A}} \tag{32}$$

- Exponential of an operator:

$$e^{\hat{A}} = 1 + \hat{A} + \frac{1}{2}\hat{A}^2 + \cdots + \frac{1}{k!}\hat{A}^k + \cdots \tag{33}$$

Please note

$$e^{\hat{A}} e^{\hat{B}} \neq e^{\hat{A}+\hat{B}} \tag{34}$$

if $[\hat{A}, \hat{B}] \neq 0$.

Unitary transformation

Suppose

$$\hat{A}|a_n\rangle = a_n|a_n\rangle. \tag{35}$$

Given a unitary operator $\hat{U}$, we have

$$\hat{U}\hat{A}\hat{U}^\dagger(\hat{U}|a_n\rangle) = a_n(\hat{U}|a_n\rangle) \tag{36}$$

This means $\hat{A}' \equiv \hat{U}\hat{A}\hat{U}^\dagger$ share the same eigenvalues with $\hat{A}$. Therefore,

$$\mathrm{Tr}\,\hat{A} = \mathrm{Tr}\,\hat{A}' \quad \text{and} \quad \det\hat{A} = \det\hat{A}' \tag{37}$$

Schrödinger equation

The time evolution equation for a quantum state:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{38}$$

Here $\hat{H}$ is the Hamiltonian of a system. The formal solution of the system is given by

$$|\psi(t)\rangle = e^{-i\hat{H}(t-t_0)/\hbar}|\psi(t_0)\rangle \tag{39}$$

If the Hamiltonian satisfies

$$\hat{H}|n\rangle = E_n|n\rangle \tag{40}$$

we have

$$|\psi(t)\rangle = \sum_n e^{-iE_n(t-t_0)/\hbar}\langle n|\psi(t_0)\rangle|n\rangle \tag{41}$$

Schrödinger equation

How to solve a Schrödinger equation systematically? Suppose the Hamiltonian is expressed under one representation, e.g.,

$$\hat{H} = \sum_{mn} H_{mn} |a_m\rangle\langle a_n| \Longrightarrow \mathbf{H} \tag{42}$$

Method I:

1. Diagonalize the Hamiltonian and obtain E_n and $|n\rangle$;
2. Expand the initial state with respect to $|n\rangle$;
3. Use Eq. (41) to obtain the solution.

Method II:

1. Calculate $e^{-i\hat{H}t/\hbar}$ directly;
2. In one representation,

$$e^{\mathbf{A}} = e^{\mathbf{U}\mathbf{U}^{-1}\mathbf{A}\mathbf{U}\mathbf{U}^{-1}} = e^{\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{-1}} = \mathbf{U}e^{\mathbf{\Lambda}}\mathbf{U}^{-1} \tag{43}$$

Continuous cases

The most general Hamiltonian of a magnetic field–free system is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{44}$$

where $\hat{x}$ and $\hat{p}$ are the coordinate and momentum respectively, m is the mass, and V is the potential energy. Here we assume the system has only one degree of freedom. In this case $\hat{x}$ and $\hat{p}$ have infinite continuous number of eigenvalues. The eigenvectors are defined as

$$\hat{x}|x\rangle = x|x\rangle \quad \text{and} \quad \hat{p}|p\rangle = p|p\rangle \tag{45}$$

The orthonormality and completeness read (take x as an example)

$$\langle x|x'\rangle = \delta(x - x'), \tag{46}$$

$$1 = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x| \tag{47}$$

Coordinate and momentum

Assume the coordinate representation of $|p\rangle$ is given by

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{48}$$

Then

$$\langle x|\hat{p}|p\rangle = \int \mathrm{d}x' \, \langle x|\hat{p}|x'\rangle\langle x'|p\rangle = p\langle x|p\rangle \tag{49}$$

That is

$$\hat{p} = \int \mathrm{d}x \, |x\rangle(-i\hbar)\frac{\partial}{\partial x}\langle x| \tag{50}$$

Equivalently, we have

$$\hat{p}|x\rangle = i\hbar\frac{\partial}{\partial x}|x\rangle \tag{51}$$

For $\hat{x}$, one could also prove

$$\hat{x} = \int \mathrm{d}p \, |p\rangle(i\hbar)\frac{\partial}{\partial p}\langle p| \tag{52}$$

or

$$\hat{x}|p\rangle = -i\hbar\frac{\partial}{\partial p}|p\rangle \tag{53}$$

Coornidate and momentum

The Heisenberg's commutator relation reads

$$[\hat{x}, \hat{p}] = i\hbar \tag{54}$$

Prove:

$$\hat{x}\hat{p} = \int \mathrm{d}x\, x|x\rangle(-i\hbar)\frac{\partial}{\partial x}\langle x|$$
$$\hat{p}\hat{x} = \int \mathrm{d}x\, x|x\rangle(-i\hbar)\frac{\partial}{\partial x}\langle x| - i\hbar \cdot 1$$

The commutator relation can be generalized as

$$[\hat{x}, f(\hat{p})] = i\hbar\frac{\partial}{\partial p}f(p)\bigg|_{p=\hat{p}} \quad \text{and} \quad [\hat{p}, f(\hat{x})] = -i\hbar\frac{\partial}{\partial x}f(x)\bigg|_{x=\hat{x}} \tag{55}$$

The notable wave function is defined as the combination coefficient of one quantum state $|\psi\rangle$ expanded in the coordinate representation, that is,

$$\psi(x,t) \equiv \langle x|\psi(t)\rangle \tag{56}$$

The correspondence Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial x}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t) \tag{57}$$

Coornidate and momentum

In the momentum representation, the wave function is defined as

$$\tilde{\psi}(p,t) \equiv \langle p|\psi(t)\rangle \tag{58}$$

It can be also obtained from $\psi(x,t)$ via unitary transformation reading

$$\tilde{\psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}x\, e^{-ipx/\hbar} \psi(x,t) \tag{59}$$

Or inversely

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \mathrm{d}p\, e^{ipx/\hbar} \tilde{\psi}(p,t) \tag{60}$$

The inner product reads

$$\langle\psi|\varphi\rangle = \int \mathrm{d}x\, \psi^*(x)\varphi(x) = \int \mathrm{d}p\, \tilde{\psi}^*(p)\tilde{\varphi}(p) \tag{61}$$

And also

$$\langle\psi|f(\hat{x})|\varphi\rangle = \int \mathrm{d}x\, \psi^*(x)f(x)\varphi(x) = \int \mathrm{d}p\, \tilde{\psi}^*(p)f\Big(i\hbar\frac{\partial}{\partial p}\Big)\tilde{\varphi}(p) \tag{62}$$

$$\langle\psi|f(\hat{p})|\varphi\rangle = \int \mathrm{d}x\, \psi^*(x)f\Big(-i\hbar\frac{\partial}{\partial x}\Big)\varphi(x) = \int \mathrm{d}p\, \tilde{\psi}^*(p)f(p)\tilde{\varphi}(p) \tag{63}$$

Unitary operator

Prove $e^{i\lambda\hat{A}}$ is unitary, with $\lambda \in \mathbb{R}$ and $\hat{A} = \hat{A}^\dagger$
Firstly,

$$(e^{i\lambda\hat{A}})^\dagger = e^{-i\lambda\hat{A}} \tag{64}$$

Secondly,

$$e^{i\lambda\hat{A}}e^{-i\lambda\hat{A}} = \; e^{i(\lambda-\lambda)\hat{A}} = 1? \tag{65}$$

Since $[\hat{A}, \hat{A}] = 0$, we could treat the above equality the same as the c-number case, that is, the equality holds.
Rigorous proof: Define

$$\hat{C} \equiv e^{i\lambda\hat{A}}e^{-i\lambda\hat{A}} \tag{66}$$

Then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\hat{C} = i[\hat{A}, \hat{C}] = 0 \tag{67}$$

Therefore, $\hat{C} = \mathrm{const} \cdot 1$. According to $\hat{C}(\lambda = 0) = 1$, we prove the result.

Unitary operator

FYI:

$$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}] + \frac{1}{2}[\hat{A},[\hat{A},\hat{B}]] + \cdots + \frac{1}{k!}\underbrace{[\hat{A},[\hat{A}\cdots,[\hat{A},}_{k\,\mathrm{th}}\hat{B}]\cdots]] + \cdots \tag{68}$$

FYI:

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{C}} \tag{69}$$

with

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A},\hat{B}] + \frac{1}{12}[\hat{A},[\hat{A},\hat{B}]] - \frac{1}{12}[\hat{B},[\hat{A},\hat{B}]] + \cdots \tag{70}$$

Two state system

Consider the system with Hamiltonian

$$\hat{H} = \beta(|1\rangle\langle 2| + |2\rangle\langle 1|) \tag{71}$$

where $\beta \in \mathbb{R}$ and $\langle a|b\rangle = \delta_{ab}$ $(a, b = 1, 2)$.

- Diagonalize the Hamiltonian.

$$\hat{H} \Longrightarrow \mathbf{H} = \begin{bmatrix} 0 & \beta \\ \beta & 0 \end{bmatrix} \tag{72}$$

The characteristic equation gives eigenvalues being

$$E_{\pm} = \pm\beta \tag{73}$$

And the eigenvalues are

$$\psi_+ = \frac{1}{\sqrt{2}}[1, 1]^T \Longrightarrow \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \equiv |+\rangle \tag{74}$$

$$\psi_- = \frac{1}{\sqrt{2}}[1, -1]^T \Longrightarrow \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \equiv |-\rangle \tag{75}$$

Two state system

- Given initial state $|\psi(0)\rangle = |1\rangle$, then we have

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar}|1\rangle = e^{-i\beta t/\hbar}|+\rangle\langle+|1\rangle + e^{i\beta t/\hbar}|-\rangle\langle-|1\rangle$$
$$= \cos(\beta t/\hbar)|1\rangle - i\sin(\beta t/\hbar)|2\rangle \quad (76)$$

Oscillate between $|1\rangle$ and $|2\rangle$ with frequency $\Omega = \frac{\pi\hbar}{2|\beta|}$.

- The inner product:

$$\langle\psi(t)|\psi(t)\rangle = 1 \quad (77)$$

If $\operatorname{Im}\beta \neq 0$, we have

$$\langle\psi(t)|\psi(t)\rangle = \cosh(2\operatorname{Im}\beta t/\hbar) \neq 1 \quad (78)$$