

transformation law for matrices and vectors.

Linear Vector Spaces and Quantum Mechanics (Ref: Sakurai)

So far we have seen formal defns of vector space. For the rest of the discussions, we will connect its importance to Quantum Mechanics.

- The state of a system is represented by a state vector in a complex vector space. Such a state is denoted by $|\alpha\rangle$ and is called a ket. α : represents any information that is required to know its state.
- Following rules of LVS:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \quad (|\alpha\rangle, |\beta\rangle, |\gamma\rangle \in S)$$

$$c|\alpha\rangle = |\alpha\rangle \quad (c \in \text{Complex number})$$

$|\alpha\rangle, c|\alpha\rangle$ represents the same physical state.
etc.

- The dimensionality of the LVS is specified by the system under consideration by the number of quantum-mechanical degrees of freedom.

Ex: Spin $\frac{1}{2} \rightarrow$ has 2 degrees of freedom $\uparrow \downarrow \Rightarrow N=2$

\vec{p} : infinite degrees of freedom $\Rightarrow N=\infty$

\vec{x} : $N=\infty$

Infinite dim. VS with Norm defined is called a Hilbert space (HS)

- Any measurement made gives us an observable.
An observable is represented by an operator such as \hat{A} . (already seen that operators form a VS and ones of interest satisfy linearity condition $\hat{A}(|\alpha\rangle + |\beta\rangle) = \hat{A}|\alpha\rangle + \hat{A}|\beta\rangle$)

- Operator acts on a ket $|\alpha\rangle$:

$$\hat{A} \cdot |\alpha\rangle = \hat{A}|\alpha\rangle \equiv |\beta\rangle \quad (|\alpha\rangle, |\beta\rangle \in S \rightarrow \text{for simplicity})$$

- If $\hat{A}|\alpha\rangle = a|\alpha\rangle$ where a : complex constant
Then $|\alpha\rangle \equiv$ eigenket of \hat{A} , a is an eigenvalue eqn,
& a : eigenvalue of \hat{A} .

- Eigenkets of \hat{A} forms a basis in an N dimensional space.

$$\Rightarrow |\alpha\rangle = \sum_{a'} c_{a'} |\alpha'\rangle$$

$c_{a'}$: Complex coeffs. \rightarrow Already seen that this expansion is unique.

- Dual vectors: Bra $|\alpha\rangle \leftrightarrow \langle\alpha|$
 $c|\alpha\rangle \leftrightarrow \langle\alpha|c^*$

- Inner prod: $\langle\alpha| \cdot |\beta\rangle = \langle\alpha|\beta\rangle \equiv$ Complex number

Properties: $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$ (Complex conjugates)

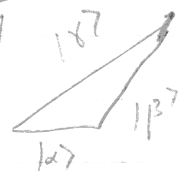
- $\langle\alpha|\alpha\rangle \geq 0$ (Real)

- Norm = $\sqrt{\langle\alpha|\alpha\rangle} \rightarrow$ length of vector

- Satisfies triangle inequality

$$\sqrt{\langle\alpha|\alpha\rangle} \leq \sqrt{\langle\alpha|\alpha\rangle} + \sqrt{\langle\beta|\beta\rangle}$$

$$|\gamma\rangle = |\alpha\rangle + |\beta\rangle$$



\Rightarrow Inner pdts: defines distances

• Adjoint of an operator X^\dagger

$$\overline{\langle \alpha | X | \beta \rangle} = \langle \beta | X^\dagger | \alpha \rangle$$

Usually $X \neq X^\dagger$

- If $X = X^\dagger$: Hermitian.

- If $X^\dagger = X^{-1}$: Unitary (preserves Norm).

• $X \neq YX$ X, Y are operators

• Outer prod: $|\alpha\rangle, |\beta\rangle$ es

$$|\alpha\rangle\langle\beta| \equiv \hat{O} \quad \text{Defn of outer product.}$$

• Eigenkets as observables:

Usually in quantum mechanics, Hermitian op. of interest turn out to be operators representing some physical observable.

• A Hermitian operator has real eigenvalues and the corresponding kets are orthogonal.

$$\begin{aligned} \text{Proof: } A|a'\rangle &= a'|a'\rangle & * \rightarrow \text{left mply by } \langle a''| \\ \langle a''|A &= a''^* \langle a''| & \rightarrow \text{rt. mltply by } |a'\rangle \end{aligned}$$

$$\therefore \langle a''|A|a'\rangle = a' \langle a''|a'\rangle = a''^* \langle a''|a'\rangle$$

$$\therefore (a' - a''^*) \langle a''|a'\rangle = 0$$

$$\Rightarrow \text{if } a' = a''^* \text{ if } a'' = a'$$

$$\text{if } a'' \neq a', \quad \langle a''|a'\rangle = 0 \quad (\text{orthogonality})$$

$$\langle a'' | a' \rangle = \underbrace{\delta_{a'' a'}}_{\text{Kronecker delta}} = \begin{cases} 1 & \text{if } a' = a'' \\ 0 & \text{otherwise} \end{cases}$$

• Eigenkets as Base kets:

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle$$

$$\begin{aligned} \text{Then: } \langle a'' | \alpha \rangle &= \sum_{a'} c_{a'} \underbrace{\langle a'' | a' \rangle}_{\delta_{a'' a'}} \\ &= c_{a''} \end{aligned}$$

$\Rightarrow c_a = \langle a | \alpha \rangle$ are the expansion coeffs.

$$\begin{aligned} \therefore |\alpha\rangle &= \sum_{a'} \langle a' | \alpha \rangle |a'\rangle \\ &= \sum_{a'} |a'\rangle \langle a' | \alpha \rangle \end{aligned}$$

(Analogous to: $\vec{v} = \sum_i \hat{e}_i (\hat{e}_i \cdot \vec{v})$)

$$|\alpha\rangle = \underbrace{\left(\sum_{a'} |a'\rangle \langle a'| \right)} \cdot |\alpha\rangle$$

$$\sum_{a'} |a'\rangle \langle a'| = \mathbb{1} \quad \text{since } |\alpha\rangle \text{ is arbitrary.}$$

Identity operator

Completeness relation or closure.

We can use $\sum_{a'} |a'\rangle \langle a'| = \mathbb{1}$ as a trick too:

$$\begin{aligned} \text{Now: } \langle \alpha | \alpha \rangle &= \sum_{a'} \langle \alpha | a' \rangle \langle a' | \alpha \rangle = \sum_{a'} |\langle a' | \alpha \rangle|^2 \\ &= \sum_{a'} |c_{a'}|^2 \end{aligned}$$

\Rightarrow if $\langle \alpha | \alpha \rangle = 1$, then: $\sum_{a'} |c_{a'}|^2 = 1$

Completeness relation can be written in terms of projection operator:

$$P_{a'} = |a'\rangle \langle a'|$$

$$\Rightarrow \sum_{a'} P_{a'} = 1$$

• Matrix Representation of operators:

$$\hat{X} = \sum_{a'} \sum_{a''} |a''\rangle \langle a'' | \hat{X} | a'\rangle \langle a'|$$

N^2 numbers of the form: $\langle a'' | \hat{X} | a'\rangle \equiv$ Matrix.

row column

$$X \equiv \begin{pmatrix} \langle a^{(1)} | X | a^{(1)} \rangle & \langle a^{(1)} | X | a^{(2)} \rangle & \dots \\ \langle a^{(2)} | X | a^{(1)} \rangle & \langle a^{(2)} | X | a^{(2)} \rangle & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

$X^\dagger \equiv$ Complex conjugate transpose of X .

$$\bullet | \gamma \rangle = X | \alpha \rangle$$

$$\begin{aligned} \text{So } \langle a' | \gamma \rangle &= \langle a' | X | \alpha \rangle \\ &= \sum_{a''} \langle a' | X | a'' \rangle \langle a'' | \alpha \rangle \end{aligned}$$

vector \equiv Matrix \times Vector.

- What happens if the operator is diagonal?
- How does the outer prod. look in a Matrix representation?

Measurement Observables and Uncertainty relation

We have ~~to~~ already some notions of this informally by trying to observe an e^- passing through a 2 slit diffraction set up. (Diffraction pattern collapses). Let us now formally discuss measurements.

- A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured.

- i.e. Before a measurement, the state is $|\alpha\rangle$. If $\{|a'\rangle\}$ are the eigenkets of the operator \hat{A} (observable being measured), then:

$$|\alpha\rangle = \sum_{a'} c_{a'} |a'\rangle = \sum_{a'} |a'\rangle \langle a'|\alpha\rangle$$

When a measurement of \hat{A} is made, $|\alpha\rangle \longrightarrow |a'\rangle$

\Rightarrow Measurement changes the state of the system

Exception: If the system is already in an eigenstate of \hat{A} , then it continues to be so after the measurement.

- This is how when an observable is measured, we get one of its eigenvalues.

- A priori, we do not know which of $\{|a'\rangle\}$, the system is going to collapse into, but we know the prob. of this happening:
 $|c_{a'}|^2 = \text{Prob. of getting } a'$

- Expectation value of \hat{A}

$$\langle A \rangle = \langle \alpha | A | \alpha \rangle \quad (\text{Defn}).$$

(26)

$$= \sum_{a' a''} \langle \alpha | a' \rangle \langle a' | A | a'' \rangle \langle a'' | \alpha \rangle$$

$$= \sum_{a' a''} \langle \alpha | a' \rangle a' \delta_{a' a''} \langle a'' | \alpha \rangle$$

$$= \sum_{a'} a' \underbrace{|\langle \alpha | a' \rangle|^2}_{\text{Prob. of getting } a'}$$

→ Agrees with our notion of average measured value.

• Commuting Operators:

If \hat{A} and \hat{B} are 2 observables (denoted here by operators), then in general:

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}.$$

$$\text{or: } [\hat{A}, \hat{B}] \neq 0$$

\hat{A}, \hat{B} are said to be non-commuting.

• If $[\hat{A}, \hat{B}] = 0$, then \hat{A}, \hat{B} are commuting observables.

The eigenkets of \hat{A} and \hat{B} share very interesting relationship.

$$\text{Let } \hat{A}|a\rangle = a|a\rangle$$

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

Thm: If $[A, B] = 0$ and \hat{A} is diagonal, and eigenvalues are non-degenerate, then matrix elements of $\langle a'' | B | a' \rangle$ is also diagonal.

$$\text{Proof: } \langle a'' | [A, B] | a' \rangle = \langle a'' | AB | a' \rangle - \langle a'' | BA | a' \rangle$$

$$= (a'' - a') \langle a'' | B | a' \rangle = 0$$

$$\text{If } a' \neq a'', \text{ then } \langle a'' | B | a' \rangle = 0$$

• Degeneracy: If two eigenkets of \hat{A} have the same eigenvalue, then the eigenkets are degenerate and one cannot distinguish the two. Most of the earlier theorems: Orthogonality, existence of basis (linear indep) was proved on the basis that no two eigenvalues are the same. In quantum mechanics, this usually implies that $|a\rangle$ alone does not sufficiently describe the system, and usually another label, usually the eigenvalue of some other commuting observable can be used to label them.

• Going back to commuting observables:

$$\langle a'' | B | a' \rangle = \delta_{a'a''} \langle a' | B | a' \rangle$$

Since A, B can be represented using the same kets:

$$B | a' \rangle =$$

$$B = \sum_{a''} | a'' \rangle \langle a'' | B | a' \rangle \langle a'' |$$

$$\Rightarrow B | a' \rangle = \sum_{a''} | a'' \rangle \langle a'' | B | a' \rangle \langle a'' | a' \rangle$$

$$= \underbrace{\langle a' | B | a' \rangle}_{b} | a' \rangle$$

$b \rightarrow$ eigenvalue of \hat{B} .

$\therefore \{ | a' \rangle \}$: simultaneous eigenkets of \hat{A} and \hat{B} .

• What happens if there is n -fold degeneracy?

$$\text{i.e. } A | a^{(i)} \rangle = a' | a^{(i)} \rangle \quad i=1, 2, \dots, n$$

$| a^{(i)} \rangle$ are n mutually orthogonal kets of A with the same eigenvalue a' . Choose appropriate linear combination and

diagonalize B in that basis. Therefore $[A, B] = 0 \Rightarrow \hat{A}, \hat{B}$ share the same eigenkets. If $|a', b'\rangle$ are the eigenkets of \hat{A}, \hat{B} , then:

$$\hat{A}|a', b'\rangle = a'|a', b'\rangle$$

$$\hat{B}|a', b'\rangle = b'|a', b'\rangle$$

This notation is particularly useful if there is degeneracy, and is superfluous if there isn't any.

Example: Orbital angular momentum, need l, m_z to specify the state completely.

- Can use a collective index $|k'\rangle$ to stand for $|a', b'\rangle \dots$

i.e.: $|k'\rangle = |a', b'\rangle$

- We can generalize to a situation where there are several commuting operators.

$$[A, B] = [B, C] = [A, C] = \dots = 0$$

Once we have this maximal set of commuting observables, we form eigenkets (basis) by using all the eigenvalues as labels. While some of the operators can have degeneracies, these get lifted by other labels. Then:

$$|k'\rangle = |a', b', c', \dots\rangle$$

$$\langle k'' | k' \rangle = \delta_{a'a''} \delta_{b'b''} \delta_{c'c''} \dots$$

$$\sum_{k'} |k'\rangle \langle k'| = \sum_{a', b', c', \dots} |a', b', c', \dots\rangle \langle a', b', c', \dots|$$

- What happens to measurements?

When \hat{A} is measured we get the result ~~the~~ a' , measuring B gives b' and if A is measured again, we still get a' by defn. Therefore measurements do not affect the state of the system.

Non-commuting observables and measurements:

• These do not have simultaneous eigenkets.

Proof: If $[A, B] \neq 0$, and if they had simultaneous eigenkets, then:

$$AB|a', b'\rangle = a'b'|a', b'\rangle$$

$$BA|a', b'\rangle = a'b'|a', b'\rangle$$

$\Rightarrow AB = BA$ which is not true. — Q.E.D.

• It is possible that there is a subspace where $[A, B] = 0$.
→ Will see this later with angular momentum.

• A measurement will affect the state of the system. (Reminder)
Recall: Interference exp't with light source to detect e^- passing through hole 1 or 2.

Uncertainty Relation:

We have seen this as a fundamental axiom in q-mech. We will now formally establish this.

Given an observable A , we define:

$$\Delta A = A - \langle A \rangle \text{ (operator)}$$

where the expectation value is taken for a certain physical state under consideration.

~~$$\begin{aligned} \langle \Delta A \rangle^2 &= \langle A - \langle A \rangle \rangle^2 \\ &= \langle A \rangle^2 + \langle A \rangle^2 - 2A \end{aligned}$$~~

$$\langle (\Delta A)^2 \rangle = \langle (A - \langle A \rangle)^2 \rangle$$

$$= \langle A^2 - 2A\langle A \rangle + \langle A \rangle^2 \rangle$$

$$= \langle A^2 \rangle - 2\langle A \rangle^2 + \langle A \rangle^2$$

$$= \langle A^2 \rangle - \langle A \rangle^2$$

dispersion / variance / mean sq. deviation

- If $|\psi\rangle$ is an eigenstate of A , then $\langle (\Delta A)^2 \rangle = 0$.
- dispersion of an observable characterizes its fuzziness.

• Statement of Uncertainty:

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

We prove this in the following steps:

(i) Schwarz inequality:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2 \quad (|\vec{a}|^2 |\vec{b}|^2 \geq |\vec{a} \cdot \vec{b}|^2)$$

Proof:

Define: $|\alpha\rangle + \lambda |\beta\rangle$

λ : Complex number.

$$\text{Then: } (\langle \alpha | + \lambda^* \langle \beta |) \cdot (|\alpha\rangle + \lambda |\beta\rangle)$$

$$= \langle \alpha | \alpha \rangle + \lambda \langle \alpha | \beta \rangle + \lambda^* \langle \beta | \alpha \rangle + \lambda |\langle \beta | \beta \rangle|$$

The inner prod ≥ 0 .

$$\therefore \langle \alpha | \alpha \rangle + \lambda \langle \alpha | \beta \rangle + \lambda^* \langle \beta | \alpha \rangle + \lambda |\langle \beta | \beta \rangle| \geq 0$$

Since λ is arbitrary, set

$$\lambda = - \frac{\langle \beta | \alpha \rangle}{\langle \beta | \beta \rangle}$$

$$\langle \alpha | \alpha \rangle - \frac{\langle \beta | \alpha \rangle \langle \alpha | \beta \rangle}{\langle \beta | \beta \rangle} + \frac{\langle \alpha | \beta \rangle \langle \beta | \alpha \rangle}{\langle \beta | \beta \rangle} + \frac{|\langle \beta | \alpha \rangle|^2}{\langle \beta | \beta \rangle} \geq 0$$

$$\text{or: } \langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \beta | \alpha \rangle|^2$$

• We know that the expectation value of a Hermitian operator is purely real.

• If $c = -c^\dagger$ (Anti Hermitian) then let us determine its expectation value:

$$\langle c | c | c' \rangle = \langle c | c' \rangle c'$$

$$\langle c | c^\dagger | c' \rangle = c'^* \langle c' | c \rangle$$

Then:

$$\text{If } c = -c^\dagger$$

$$\text{Then: } c' = -(c')^*$$

$$c' = ib$$

$$\text{Then } (c')^* = -ib$$

$$\text{Then: } c' = -(c')^*$$

\Rightarrow expectation value is purely imaginary.

Define:

$$|\alpha\rangle = \Delta A | \rangle$$

$$|\beta\rangle = \Delta B | \rangle$$

Using Schwarz inequality:

$$\langle \alpha | \alpha \rangle \langle \beta | \beta \rangle \geq |\langle \alpha | \beta \rangle|^2$$

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

$$\Delta A \Delta B = \frac{1}{2} [\Delta A, \Delta B] + \frac{1}{2} \{ \Delta A, \Delta B \}$$

Check:

$$\underbrace{\frac{1}{2} [\Delta A, \Delta B]}_{\text{Anti-commutator}}$$

$$= \frac{1}{2} (\Delta A \Delta B - \Delta B \Delta A) + \frac{1}{2} (\Delta A \Delta B + \Delta B \Delta A)$$

$$= \Delta A \Delta B$$

Let us evaluate

$$[\Delta A, \Delta B] = [A - \langle A \rangle, B - \langle B \rangle] = [A, B]$$

$$\begin{aligned}
 [A, B]^{\dagger} &= (AB - BA)^{\dagger} \\
 &= B^{\dagger} A^{\dagger} - A^{\dagger} B^{\dagger} \\
 &= BA - AB \\
 &= -[A, B].
 \end{aligned}$$

⇒ [A, B] is anti-Hermitian, while {A, B} is Hermitian.

$$\Rightarrow \langle \Delta A \Delta B \rangle = \frac{1}{2} \underbrace{\langle [A, B] \rangle}_{\text{pure imag.}} + \frac{1}{2} \underbrace{\langle \{A, B\} \rangle}_{\text{pure real.}}$$

$$\therefore |\langle \Delta A \Delta B \rangle|^2 = \frac{1}{4} |\langle [A, B] \rangle|^2 + \frac{1}{4} \underbrace{|\langle \{A, B\} \rangle|^2}_{\text{usually omitted.}}$$

$$\therefore \langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} |\langle [A, B] \rangle|^2 \quad (\text{Makes it stronger})$$

Change of basis:
If [A, B] ≠ 0

- ⇒ The space can be spanned either by the kets of A or B.
- See how to transform from one basis to the other.
- Change of basis or change of representation

Thm: Given two set of basis states, (orthonormal, complete), there exists a unitary operator U such that
 $|b^{(1)}\rangle = U|a^{(1)}\rangle, |b^{(2)}\rangle = U|a^{(2)}\rangle \dots$

where:

$$\begin{aligned}
 U^{\dagger} &= U^{-1} \\
 \text{and } U U^{\dagger} &= U^{\dagger} U = 1
 \end{aligned}$$

$$U = \sum_k |a^{(k)}\rangle \langle b^{(k)}|$$

Considers: $U = \sum_k |b^{(k)}\rangle \langle a^{(k)}|$

$$\begin{aligned}
 U^{\dagger} U &= \sum_{k, k'} |a^{(k)}\rangle \langle b^{(k)}| \langle b^{(k')}| \langle a^{(k')}| \\
 &= \sum_k |a^{(k)}\rangle \langle a^{(k)}| \delta_{kk'} = 1
 \end{aligned}$$

$$\text{Then: } U|a^{(l)}\rangle = \sum_k |b^{(k)}\rangle \underbrace{\langle a^{(k)} | a^{(l)} \rangle}_{\delta_{kl}} \\ = |b^{(l)}\rangle$$

→ Why should this transf. be unitary?

Matrix Representation of U:

$$\langle a^{(k)} | U | a^{(l)} \rangle = \sum_m \langle a^{(k)} | b^{(m)} \rangle \underbrace{\langle a^{(m)} | a^{(l)} \rangle}_{\delta_{ml}} \\ = \langle a^{(k)} | b^{(l)} \rangle$$

Matrix elements are the inner prod of old base bra, and new base kets.

• An arbitrary vector

$$|\alpha\rangle = \sum_a |a^{(l)}\rangle \underbrace{\langle a^{(l)} | \alpha \rangle}_{c_a}$$

$$\langle b^{(k)} | \alpha \rangle = c_{b^{(k)}} = \sum_l \langle b^{(k)} | a^{(l)} \rangle \langle a^{(l)} | \alpha \rangle$$

$$\text{But } \langle b^{(k)} | = \langle a^{(k)} | U^\dagger$$

$$\Rightarrow \langle b^{(k)} | \alpha \rangle = \sum_l \langle a^{(k)} | U^\dagger | a^{(l)} \rangle \langle a^{(l)} | \alpha \rangle$$

$$\Rightarrow \text{New} = U^\dagger(\text{old})$$

and for the operators:

$$X' = U^\dagger X U \longrightarrow \text{Similarity Transf.}$$

Diagonalization:

$\hat{B}|a'\rangle = |a'\rangle$ (not number times $|a'\rangle$).
But there exists a basis $\{|b'\rangle\}$:

$$\hat{B}|b'\rangle = b'|b'\rangle$$

$$\sum_{a'} \hat{B}|a'\rangle \langle a'|b'\rangle = b'|b'\rangle$$

$$\sum_{a'} \langle a''|\hat{B}|a'\rangle \langle a'|b'\rangle = b' \langle a''|b'\rangle$$

Written out in terms of a matrix eqn:

$$\begin{pmatrix} B_{11} & B_{12} & \dots \\ B_{21} & B_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1^{(b')} \\ c_2^{(b')} \\ \vdots \end{pmatrix} = b^{(b')} \begin{pmatrix} c_1^{(b')} \\ c_2^{(b')} \\ \vdots \end{pmatrix}$$

$|b^{(k)}\rangle \equiv \lambda^{(k)}$ eigenvalue.

N base kets: N eigenvalues and for each eigenvalue 1 eigenvector (N components).

Solution exists iff: $|B - \lambda I| = 0 \rightarrow$ linear algebra
 \rightarrow Can you prove this?

Unitary Equivalent Observables:

\Rightarrow Thm: Consider two sets of orthonormal basis $\{|a'\rangle\}$ and $\{|b'\rangle\}$ connected by the U operator. The operator A and UAU^{-1} are said to be unitary equivalent observables.

Now:

$$A|a^{(k)}\rangle = a^{(k)}|a^{(k)}\rangle$$

$$\Rightarrow UAU^{-1}U|a^{(e)}\rangle = a^{(e)}U|a^{(e)}\rangle$$

$$\Rightarrow [UAU^{-1}]|b^{(e)}\rangle = a^{(e)}|b^{(e)}\rangle$$

Eigenvalue is preserved.