Beginner's Guide to Quantum Mechanics

- Notes on Nielsen's Quantum Computation and Quantum Information Chpt II, and YouTube tutorial "Math of Quantum Mechanics" by Quantum Sense
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Contents

1 vector space

- C^n: space of all n-tuple complex numbers (c numbers)

i.e. $(z_1, z_2, z_3, ..., z_n)$

- a vector space is closed under scalar multiplicationa nd addition

1.1) Dirac notation

Symbols	**Meaning**
$\lvert v\rangle$	ket, a vector in vec space
$\langle v\rvert$	bra, a dual vector in vec space; the complex transpose of ket $\langle v\rvert = (\lvert v\rangle^*)^\top$
$\langle v\lvert w\rangle$	inner product of $\lvert v\rangle$ and $\lvert w\rangle$
$\lvert\varphi\rangle \otimes \lvert\psi\rangle$	tensor product of $\lvert\varphi\rangle$ and $\lvert\psi\rangle$ abbriviates as $\lvert\varphi\rangle\lvert\psi\rangle$
$\boldsymbol{A}^*$	complex conjugate of $\boldsymbol{A}$
$\boldsymbol{A}^\top$	transpose of $\boldsymbol{A}$
$\boldsymbol{A}^\dagger$	hermitian conjugate of $\boldsymbol{A}$ i.e. $\boldsymbol{A}^\dagger = (\boldsymbol{A}^*)^\top$ $$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^\dagger = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix} \quad (1)$$
$\langle\varphi\lvert\boldsymbol{A}\rvert\psi\rangle$	inner product betweeen $\lvert\varphi\rangle$ and $\boldsymbol{A}\lvert\psi\rangle$

1.2) Span

a set of bec $|v_1\rangle, |v_2\rangle, ..., |v_n\rangle$ spans the vector space if any vector in the space can be written as

$$|v\rangle = \sum_i a_i |v_i\rangle \quad (2)$$

for some complex numbers a_i

1.3) Linear Independence

a set of non-zero vectors $|v_1\rangle, |v_2\rangle, ..., |v_n\rangle$ are liinearly dependent if there exists a set of complex numbers $a_1, a_2, ..., a_n$, s.t.

$$a_1|v_1\rangle + a_2|v_2\rangle + ... + a_n|v_n\rangle = 0 \quad (3)$$

If the only solution to the above equation is $a_1 = a_2 = ... = a_n = 0$, then the vectors are **linearly independent**

1.4) Linear operators

A linear operator A is any linear function that

$$A\left(\sum_i a_i |v_i\rangle\right) = \sum_i a_i A(|v_i\rangle) \quad (4)$$

It is convention to write $A(|v_i\rangle) = A|v_i\rangle$

- Identity Operator $I_V : I_V|v\rangle \equiv |v\rangle$. It is convinent to write I if no confution arises.
- zero operator $0|v\rangle \equiv 0$
- composition of linear operators A and B is AB

We observe that the above is equivalent to the matrix representation of linear transformations.

In other words, for a linear operator $A : V \to W$, and suppose $|v_1\rangle, |v_2\rangle, ..., |v_m\rangle$

1.5) Hilbert Space

Given a vector basis $\{|E_i\rangle\}$, when attempting to represent a polynomial as $p = \sum_{i=0}^{\infty} a_i E_i$, the sum is in the form of, according to taylor series, an exponential function. But the exponential function is not a polynomial, i.e. outside of our vector space, so we have landed on a paradox. To avoid this, we define a **Hilbert Space** to handle infinite dimensional vector spaces.

- A Hilbert spsace is a vector space that is 1. complete and 2. has an inner product defined on it. In other words, every converging set of vectors must converge to an element **inside** the vector space.

$$|\psi\rangle \in \mathcal{H} \tag{5}$$

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2 Inner product

- Review on dot product
  - orthogonality & angle
  - norm $\|\vec{v}\| = \sqrt{\vec{v} \cdot \vec{v}}$

For kets $|\psi\rangle, |\varphi\rangle, |\zeta\rangle$, and scalar a, an inner product has the following rules:

- Linearity in the second argument:

$$\begin{cases} \langle\psi|\varphi + \zeta\rangle = \langle\psi|\varphi\rangle + \langle\psi|\zeta\rangle \\ \langle\psi|a\varphi\rangle = a\langle\psi|\varphi\rangle \end{cases} \tag{6}$$

- COmplex commutation:

$$\langle\psi|\varphi\rangle = \langle\varphi|\psi\rangle^* \tag{7}$$

- Positive definiteness (think of norm):

$$|\psi\rangle \neq 0 \Rightarrow \langle\psi|\psi\rangle > 0 \tag{8}$$

- Magnitude of a vector:

$$\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle} \tag{9}$$

- Orthogonality:

$$\langle\psi|\varphi\rangle = 0 \Rightarrow |\psi\rangle \text{ and } |\varphi\rangle \text{ are orthogonal} \tag{10}$$

- antilinearity in the first argument:

$$\langle a\psi + b\zeta|\varphi\rangle = a^* \langle\psi|\varphi\rangle + b^* \langle\zeta|\varphi\rangle \tag{11}$$

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3 Orthonormal basis

$\{|E_i\rangle\}$ s.t. $\langle E_i | E_j \rangle = \delta_{ij}$ is an orthonormal basis, with kroneker delta $\delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$

In English, the inner product of two vectors is 1 if they are the same (norm = 1), and 0 if they are different (orthogonal).

Using the orthonormal basis, we can write any vector as a linear combination of the basis vectors:

$$|\psi\rangle = \sum_i c_i |E_i\rangle \tag{12}$$

Notice that

$$\begin{aligned} \langle E_i|\psi\rangle &= \left\langle E_i \middle| \sum_j c_j E_j \right\rangle \\ &= \sum_j c_j \langle E_i|E_j\rangle \\ &= c_i \end{aligned} \tag{13}$$

And we use the above to calculate the coefficients c_i.

3.1) Inner product between two vectors

$$\begin{aligned} \langle \psi|\varphi\rangle &= \left\langle \sum_i c_i E_i \middle| \sum_j d_j E_j \right\rangle \\ &= \sum_i \sum_j c_i^* d_j \langle E_i|E_j\rangle \\ &= \sum_i \sum_j c_i^* d_j \delta_{ij} \\ &= \sum_i c_i^* d_i \end{aligned} \tag{14}$$

When $c, d \in \mathbb{N}$, $\langle \varphi|\psi\rangle = \sum_i c_i d_i$ is simply the dot product.

4 Continuous basis

In a Hilbert space, we can represent continuous functions as a linear combination of a set of continous basis $\{|x\rangle|\ x \in R\}$. The mathematicians said so and we do not question the validity of this argument on our own.

An example would be

$$|\psi\rangle = \int \mathrm{d}x\ c(x)\ |x\rangle \tag{15}$$

Where $c(x)$ is a function that maps x to the coefficient $c(x)$.

4.1) representatio of continuous orthonormal basis

Similar to the discrete case, we can represent the continuous orthonormal basis $\{|x\rangle|\ x \in \mathbb{R}\}$ as:

$$\langle x_i|x_j\rangle = \delta(x_i - x_j) \tag{16}$$

where $\delta(x_i - x_j)$ is the Dirac delta function. We can be pragmatic and understand the Dirac Delta function as ANY function that satisfies the following properties:

$$\begin{gathered} \int \mathrm{d}x\ f(x)\delta(c-x) = f(c) \\ \delta(c-x) = \begin{cases} 1 & x = c \\ 0 & x \neq c \end{cases} \end{gathered} \tag{17}$$

4.2) Inner product between two continuous vectors

$$
\begin{aligned}
\langle\psi|\varphi\rangle &= \left(\int \psi(x)\langle x|\,\mathrm{d}x\right)\left(\int \varphi(y)|y\rangle\,\mathrm{d}y\right) \\
&= \iint \mathrm{d}\psi^*(x)\varphi(y)\,\mathrm{d}x\,\mathrm{d}y\;\langle x|y\rangle \\
&= \int \mathrm{d}x\psi^*(x)\underbrace{\int \mathrm{d}y\varphi(y)\delta(x-y)}_{\delta\text{ property}} \\
&= \int \mathrm{d}x\psi^*(x)\;\varphi(x)
\end{aligned}
\tag{18}
$$

We have done a inner product of wavefunctions.

4.3) Finding coefficients of continuous basis

notice

$$
\begin{aligned}
\langle x_0|\psi\rangle = \langle x_0|&\left(\int \mathrm{d}x\psi(x)|x\rangle\right) \\
&= \int \mathrm{d}x\psi(x)\langle x_0|x\rangle \\
&= \int \mathrm{d}x\psi(x)\;\delta(x_0-x) \\
&= \psi(x_0)
\end{aligned}
\tag{19}
$$

So, the coefficient function $\psi(x_0) = \langle x_0|\psi\rangle$

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5 Bra and Braket notation

5.1) Linear functionals

A linear functional is a linear function that maps a vector to a scalar:

$$L\vec{v} = c, \quad c \in \mathbb{F} \tag{20}$$

L maps from the vector space to the field of scalars, or $L : \mathbb{C}^n \to \mathbb{F}$

L is actually an $1 \times n$ matrix, or a row vector.

5.2) Dual Space V^*

Set of all L, where each L is a linear funcitonal s.t. $L\boldsymbol{V} = c \in \mathbb{F}$. More rigorously we can say

$$\boldsymbol{V}^* = \{L : \boldsymbol{V} \to F \mid L \text{ is linear}\} \tag{21}$$

5.3) Bra

- $\langle\psi|$ is a shorthand of a linear functional inside a Hilbert dual space. It is an operator that when acting on a vector, will spit out a constant.

$$\langle\psi|\;|\varphi\rangle = c \in \mathbb{C} \tag{22}$$

Riesz Representation theorem

For any linear functional L_φ s.t.

$$L_\varphi\vec{v} = \mathrm{InProd}(\vec{\varphi}, \vec{v}) \tag{23}$$

where $\vec{\varphi}$ is a unique vector. In hilbert space, this unique vector is $\langle\varphi|$

So it follows that

$$\langle\varphi||\psi\rangle = \langle\varphi|\psi\rangle \tag{24}$$

5.4) Complex conjegate

Recall the fact that

$$\langle\varphi|\psi\rangle = \sum_i c_i^* d_i = \langle\varphi||\psi\rangle \tag{25}$$

where $|\varphi\rangle = \sum_i c_i |E_i\rangle$. By virtue of intuition, we can see that

$$\langle\varphi| = \left(|\varphi\rangle^*\right)^\top \tag{26}$$

5.5) Outer product

notice

$$\begin{aligned} |\psi\rangle = \sum_i c_i |A_i\rangle &= \sum_i \langle A_i|\psi\rangle\, |A_i\rangle \\ &= \sum_i |A_i\rangle\langle A_i|\psi\rangle \\ &= \sum_i |A_i\rangle\langle A_i||\psi\rangle \\ &= \left(\sum_i |A_i\rangle\langle A_i|\right)|\psi\rangle \end{aligned} \tag{27}$$

Comparing left with right, we observe that

$$\sum_i |A_i\rangle\langle A_i| = \hat{\boldsymbol{I}} \tag{28}$$

Generally, for $|a\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, |b\rangle = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ then $\langle b| = (b_1^* \;\; b_2^*)$ so

$$|a\rangle\langle b| = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}(b_1^* \;\; b_2^*) = \begin{pmatrix} a_1 b_1^* & a_1 b_2^* \\ a_2 b_1^* & a_2 b_2^* \end{pmatrix} \tag{29}$$

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6 Observables

We represent physical quantities or states as an linear operator. The genrealization of any physical state is an observable.

6.1) Linear operator

An Linear operator is a map on a vector space that preserves its original structure. i.e.,

$$\begin{cases} \widehat{\boldsymbol{M}}(|\psi\rangle + |\varphi\rangle) = \widehat{\boldsymbol{M}}|\psi\rangle + \widehat{\boldsymbol{M}}|\varphi\rangle \\ \widehat{\boldsymbol{M}}(a|\psi\rangle) = a\widehat{\boldsymbol{M}}|\psi\rangle \end{cases} \tag{30}$$

6.2) Definite stsates

Special states in which observables has one definite value. These states are eigenstates of the observable. They corresponds to eigenvalues, all possible values of the observable.

Therefore, we can represent physical states as linear combinations of the outcome eigenstates. It is intuitive to propose the following constrains:

1. Observables have real eigenvalues
2. Eigenstates span the entire vector space.
3. eigenstates are mutually orthogonal.

Thus, Eigenstates are just the basis of an observable state in disguise!

$$|\psi\rangle = \sum_i c_i |E_i\rangle \tag{31}$$

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7 Probablistic Determination of observables: Born's rule

Knowing $|\psi\rangle = \sum_i c_i |E_i\rangle$, what is probability of $|\psi\rangle$ exactly measured to be $|E_i\rangle$, i.e. $P(|\psi\rangle = E_i)$

Observe a relationship between coefficient c_i to the probability of falling into the eigenstate $|E_i\rangle$, we propose the following:

$$P(E = E_i) = f(c_i) \tag{32}$$

with intuitive constrains:

$$\begin{gathered} 1. \quad P_{\text{total}} = \sum_i f(c_i) = 1 \\ 2. \quad \left||\psi\rangle^2\right| = \sum_i^n c_i^2 = k^2 \text{ constant length of eigenstates decomposition} \end{gathered} \tag{33}$$

from 2:

$$\begin{gathered} c_1^2 + c_2^2 + \dots + c_n^2 = k^2 \\ c_n = \pm\sqrt{k^2 - a^2 - b^2 - \dots} = \pm A \end{gathered} \tag{34}$$

Obviously, linear combination is invariant under positiveness, so

$$f(c) = f(-c) \tag{35}$$

Recall property one:

$$\sum_i^n f(c_i) = 1 \tag{36}$$

$$\begin{gathered} \sum_i^{n-1} f(c_i) + f_{c_n} = 1 \\ \sum_i^{n-1} \frac{\mathrm{d}f(c_i)}{\mathrm{d}c_1} + \frac{\mathrm{d}f(c_n)}{\mathrm{d}c_1} = 0 \qquad (*) \\ \frac{\mathrm{d}}{\mathrm{d}c_1} f(c_1) - f'\left(\sqrt{k^2 - c_1^2 - c_2^2 - \dots}\right) \cdot \frac{c_1}{\sqrt{k^2 - c_1^2 \dots}} = 0 \\ \frac{1}{c_1}\frac{\mathrm{d}}{\mathrm{d}c_1} f(c_1) = \frac{f'\left(\sqrt{k^2 - c_1^2 - c_2^2 - \dots}\right)}{\sqrt{k^2 - c_1^2 - c_2^2 - \dots}} (**) \end{gathered} \tag{37}$$

Notice that if we take $\frac{\mathrm{d}}{\mathrm{d}c_2}$ on both sides at $(*)$ instead, $(**)$ becomes

$$\frac{1}{c_2}\frac{\mathrm{d}}{\mathrm{d}c_2}f(c_2) = \frac{f'\left(\sqrt{k^2 - c_1^2 - c_2^2 - \ldots}\right)}{\sqrt{k^2 - c_1^2 - c_2^2 - \ldots}} \tag{38}$$

Thus

$$\begin{gathered}
\frac{1}{c_1}\frac{\mathrm{d}}{\mathrm{d}c_1}f(c_1) = \frac{1}{c_2}\frac{\mathrm{d}}{\mathrm{d}c_2}f(c_2) \\
\frac{\mathrm{d}}{\mathrm{d}c_1}\left(\frac{1}{c_1}\frac{\mathrm{d}}{\mathrm{d}c_1}f(c_1)\right) = \frac{\mathrm{d}}{\mathrm{d}c_1}\underbrace{\left(\frac{1}{c_2}\frac{\mathrm{d}}{\mathrm{d}c_2}f(c_2)\right)}_{\text{idpt of } c_1} = 0
\end{gathered} \tag{39}$$

Integrating the first term as our apporach to this ODE:

$$f(c_1) = \frac{\lambda}{2}c_1^2 + \mu \tag{40}$$

It is obvious that we can generalize the above to any c_i,

$$f(c) = \frac{\lambda}{2}c^2 + \mu \tag{41}$$

We meditate on an initial condition:

$$f(0) = P(|\psi\rangle = 0|E_i\rangle) = 0 \tag{42}$$

This is obvious as the probability of not being in any eigenstate is 0. And we can see that $f(0) = \mu = 0$

Now recall the first constrain:

$$\sum_i f(c_i) = 1 \tag{43}$$

We exploit this constrain using the following special case to find λ

$$\begin{gathered}
f(k) + f(0) + f(0) + f(0) + \ldots = 1 \\
f(k) = 1 = \frac{\lambda}{2}k^2 \\
\Rightarrow \lambda = \frac{2}{k^2}
\end{gathered} \tag{44}$$

Collecting the above,

$$f(c) = \frac{c^2}{k^2} \tag{45}$$

We have the freedom to choose $k = 1$

Thus, we have the Born's Rule:

$$\boxed{p(E = E_i) = f(c_i) = |c_i|^2 = |\langle E_i|\psi\rangle|^2} \tag{46}$$

When applied to a continuous basis, we have the probability density funciton

$$\begin{gathered}
|\psi\rangle = \int \mathrm{d}x\psi(x)|x\rangle \\
\Rightarrow p(x) = |\psi(x)|^2
\end{gathered} \tag{47}$$

---

8 Hermitian Operator

- New notation: for a linear operator $\widehat{M}$ and vector $|\varphi\rangle$, we write

$$\begin{aligned} \widehat{M}|\varphi\rangle &= \left|\widehat{M}\varphi\right\rangle \\ \langle\psi|\widehat{M}|\varphi\rangle &= \left\langle\psi\middle|\widehat{M}\varphi\right\rangle \end{aligned} \tag{48}$$

8.1) Hermitian adjoint

We define the hermitian adjoint of an operator $\widehat{M}$ as $\widehat{M}^\dagger$, s.t.:

$$\left\langle\widehat{M}^\dagger\psi\middle|\varphi\right\rangle = \left\langle\psi\middle|\widehat{M}\varphi\right\rangle \tag{49}$$

The hermitian adjoint yields the following properties:

$$\begin{aligned} 1.\left(\widehat{M}^\dagger\right)^\dagger &= \widehat{M} \\ 2.\left(a\widehat{M} + b\widehat{N}\right)^\dagger &= a^*\widehat{M}^\dagger + b^*\widehat{N}^\dagger \\ 3.\left(\widehat{M}\widehat{N}\right)^\dagger &= \widehat{N}^\dagger\widehat{M}^\dagger \end{aligned} \tag{50}$$

8.2) Hermitian adjoint of a scalar

for a scalar c $\in \mathbb{C}$,

$$\begin{aligned} \langle\psi|c\varphi\rangle &= c\langle\psi|\varphi\rangle = \langle c^*\psi|\varphi\rangle \\ &= \left\langle c^\dagger\psi\middle|\varphi\right\rangle \\ \Rightarrow c^\dagger &= c^* \end{aligned} \tag{51}$$

the hermitian adjoint for a scalar c is its complex conjugate.

8.3) Hermitian adjoint of a ket

for kets $|\psi\rangle, |\varphi\rangle$,

$$\begin{aligned} \langle\varphi|\psi\rangle^\dagger &= \langle\varphi|\psi\rangle^* \overset{\text{comjugate symm.}}{=} \langle\psi|\varphi\rangle \\ \langle\varphi|\psi\rangle^\dagger &= (\langle\varphi|\,|\psi\rangle)^\dagger \end{aligned} \tag{52}$$

We observe that

$$\langle\psi|\,|\varphi\rangle = |\psi\rangle^\dagger\,\langle\varphi|^\dagger \tag{53}$$

We skip the proof, but it is true that

$$\begin{aligned} &|\psi\rangle^\dagger = \langle\psi| = (|\psi\rangle^*)^\top \text{ complex transpose} \\ &\langle\varphi|^\dagger = |\varphi\rangle \end{aligned} \tag{54}$$

9 Hermitian adjoint of observables

- recap on observables $\hat{E}$
  - eigenstates $|E_i\rangle$, measured values E_i
  - rules:

$$\begin{aligned} E_i &\in \mathbb{R} \\ \text{span}(|E_i\rangle) &= \boldsymbol{V} \\ \left\langle E_i\middle|E_j\right\rangle &= \delta_{ij} \end{aligned} \tag{55}$$

- Hermitian Operator: defined as any linear operator $\widehat{M}$ s.t. $\widehat{M}^\dagger = \widehat{M}$

We show below why any observable $\hat{E}$ is hermitian.

Consider an observable acting on a ket,

$$\begin{aligned} \hat{E}|\psi\rangle &= \hat{E}\sum_i c_i|E_i\rangle \\ &= \sum_i c_i\hat{E}|E_i\rangle \\ &= \sum_i c_i E_i|E_i\rangle \quad \text{(notice it's just } \boldsymbol{A}\vec{x} = \lambda\vec{x}\text{)} \\ &= \sum_i \langle E_i|\psi\rangle\ E_i|E_i\rangle \\ &= \sum_i E_i|E_i\rangle\langle E_i||\psi\rangle \end{aligned} \tag{56}$$

$$\Rightarrow \hat{E}|\psi\rangle = \left(\sum_i E_i|E_i\rangle\langle E_i|\right)|\psi\rangle$$

$$\boxed{\hat{E} = \sum_i E_i|E_i\rangle\langle E_i|}$$

Similarly, for a continuous basis, an observable $\vec{x} = \int \mathrm{d}x\ x\ |x\rangle\ \langle x|$

Now, let's find the hermitian adjoint of an observable

$$\begin{aligned} \hat{E}^\dagger &= \left(\sum_i E_i|E_i\rangle\langle E_i|\right)^\dagger \\ &= \sum_i \left(E_i|E_i\rangle\langle E_i|\right)^\dagger \\ &= \sum_i \left(|E_i\rangle\langle E_i|\right)^\dagger E_i^\dagger \\ &= \sum_i \langle E_i|^\dagger|E_i\rangle^\dagger E_i^\dagger \\ &= \sum_i \langle E_i|^\dagger|E_i\rangle^\dagger E_i^* \\ &= \sum_i E_i|E_i\rangle\langle E_i| \quad (\text{noticing } E_i^* = E_i, \text{since } E_i \in \mathbb{R}) \\ &= \hat{E} \end{aligned} \tag{57}$$

$$\boxed{\hat{E}^\dagger = \hat{E}} \tag{58}$$

We have proved that the observable $\hat{E}$ is an hermitian operator. ■

10 Commutator

- Two operators $\hat{A}, \hat{B}$ commute iff they satisfy : $\hat{A}\hat{B} = \hat{B}\hat{A}$
- Commutator: defined as $\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}$

  If $\hat{A}, \hat{B}$ are commute, then $\left\{\hat{A}, \hat{B}\right\} = 0$

Claim: Any two commutative linear operator share a simutanuous eigenbasis

Proof:

Given commutative linear operators $\hat{A}$, $\hat{B}$, and $\left[\hat{A}, \hat{B}\right] = 0$. We are to show that $\hat{A}$ and $\hat{B}$ share same eigenbasis.

Linear algebra quick fact:

Degeneracy refers to the multiplicities of eigenvalues. If a liear operator has an eigenvalue that cooresponds to N eigenvectors, we say that it is a degenerate eigenvalue with a geometric multiplicity of N. These N eigenvectors $|\varphi_i\rangle$ form an ***eigenspace*** $\left\{|\psi\rangle_i\right\}_{i=1}^{N}$ *A linear operator either has* ***degenerate eigenvalues*** *or not.*

- Let's consider when $\hat{A}$ does not have degenerate eigenvalues, i.e. each eigenvalue of $\hat{A}$ corresponds to unique eigenvectors of $\hat{A}$.

$$\hat{A}|\psi_i\rangle = \lambda_i|\psi_i\rangle \quad \text{for each } i \tag{59}$$

  Consider $\hat{B}$ acting on $|\psi_i\rangle$:

$$\hat{A}\underline{\hat{B}|\psi_i\rangle} = \hat{B}\hat{A}|\psi_i\rangle = \lambda_i \underline{\hat{B}|\psi_i\rangle} \tag{60}$$

  Notice that $\hat{B}|\psi_i\rangle$ is still an eigenvector of $\hat{A}$ with eigenvalue λ_i. Since we assumed that λ_i only corresponds to one eigenvector $|\psi_i\rangle$, $\hat{B}|\psi_i\rangle$can only be the scalar multiple of $|\psi_i\rangle$, i.e.

$$\hat{B}|\psi_i\rangle = \mu_i|\psi_i\rangle \tag{61}$$

  Notice that Equation 61 tells us that $|\psi_i\rangle$ is also the eigenvector of $\hat{B}$, with new eigenvalue μ_i.

  We have thus shown that for any eigenvector of $\hat{A}$, it is also the eigenvector of $\hat{B}$. Putting on our mathematician hats, we say: $\{|\psi_i\rangle\}_{i=1}^{N}$ also span the eigenspace of $\hat{B}$ with eigenvalues μ_i

- Now consider when $\hat{A}$ has degenrate eigenvalues, and for any degenerate eigenvalue with geometric multiplicity of k, there exsists k number of eigenvectors $|\psi\rangle$, where the eigenvectors span an eigenspace E_λ of $\hat{A}$

$$\hat{A}|\psi_i\rangle = \lambda|\psi_i\rangle \text{ for } i = 1, 2, ..., k \tag{62}$$

  Consider $\hat{B}$ acting on the eigenspace of $\hat{A}$:

$$\hat{A}\hat{B}|\psi_i\rangle = \hat{B}\hat{A}|\psi_i\rangle = \lambda\hat{B}|\psi_i\rangle \tag{63}$$

  Similar to our previous case, $\hat{E}|\psi_i\rangle \in E_\lambda$, or $\hat{B}$ preserves the eigenspace E_λ

  Notice that for any vector $|\alpha\rangle \in E_\lambda$, where E_λ is spanned by eigenvectors $|\psi_i\rangle$ corresponding to the same degenerate eigenvalue λ:

$$
\begin{aligned}
\hat{A}|\alpha\rangle &= \hat{A}\left(\sum_i^k c_i|\psi_i\rangle\right) \\
&= c_i\left(\sum_i^k \hat{A}|\psi_i\rangle\right) \\
&= c_i\left(\sum_i^k \lambda|\psi_i\rangle\right) \\
&= \lambda\left(\sum_i^k c_i|\psi_i\rangle\right) \\
&= \lambda|\alpha\rangle
\end{aligned} \tag{64}
$$

Therefore, any $|\alpha\rangle \in E_\lambda$ is an eigenvector of $\hat{A}$ with degenerate eigenvalue λ.

Spectral theorem tells us, and we take it as a fact that: $\hat{B}$ is hermitian $\Rightarrow$ it is diagnolizable on E_λ. Suppose $\{|\varphi_i\rangle\}$ is the orthonormal basis of $\hat{B}_{E_\lambda}$ (B constrained in eigenspace E), we have

$$
\hat{B}|\varphi_i\rangle = \mu|\varphi_i\rangle, \quad i = 1, 2, ..., k \tag{65}
$$

B acts in $E_\lambda \to |\varphi_i\rangle \in E_\lambda$. Equation 64 tells us that $|\varphi_i\rangle$ is an eigenvector of $\hat{A}$ as well. Noticing

$$
\hat{A}|\varphi_i\rangle = \lambda|\varphi_i\rangle \tag{66}
$$

we can state that $\{|\varphi_i\rangle\}$ is also the orthonormal basis of $\hat{A}$

Repeacing the above for every degenerate eigenvalue of $\hat{A}$, we can deduct that:

for each , $\{\varphi_{j,i}\}$, s.t. it is the simutanuous basis of (A)$\wedge\ (B)$

The union of all $\{\varphi_{j,i}\}$ forms an orthonormal basis that can simutanuously diagnolize $\hat{A}$ and $\hat{B}$

Therefore, collecting the above, we have shown that if $\left[\hat{A}, \hat{B}\right] = 0$, then they share a common eigenbasis. ■

11 Unitary operators

- A unitary operator is any linear operator whose Hermitian conjugate equals to its inverse. i.e. $\hat{U}^\dagger = \hat{U}^{-1}$
- Inner product presercation:

$$
\langle\varphi|\psi\rangle = \left\langle\hat{U}\varphi\middle|\hat{U}\psi\right\rangle \tag{67}
$$

proof:

$$
\begin{aligned}
\left\langle\hat{U}\varphi\middle|\hat{U}\psi\right\rangle &= \left\langle\hat{U}\varphi\middle|\ \hat{U}\ |\psi\right\rangle \\
&= \langle\varphi|\ \hat{U}^\dagger\ \hat{U}\ |\psi\rangle \\
&= \langle\varphi|\hat{U}^{-1}\hat{U}|\psi\rangle \\
&= \langle\varphi|\hat{I}|\psi\rangle \\
&= \langle\varphi|\psi\rangle \quad ■
\end{aligned} \tag{68}
$$

Since inner product can be considered as a generalized dot product, or a measure of the norm and angle of two vectors, we can understand unitary operators as a "**generalized rotation**" of two vectors that conserves the norm and angle between them.

- Eigenvalue has unit length:

$$|\lambda|^2 = 1 \tag{69}$$

proof: consider normalized eigenvector $|\omega\rangle$ and eigenvalue λ of $\hat{U}$. That is,

$$\begin{cases} \hat{U}|\omega\rangle = \lambda|\omega\rangle \\ \langle\omega|\omega\rangle = 1 \end{cases} \tag{70}$$

consider the following operation:

$$\left\langle \hat{U}\omega \middle| \hat{U}\omega \right\rangle = \langle\omega|\omega\rangle = 1 \tag{71}$$

$$\begin{aligned} \left\langle \hat{U}\omega \middle| \hat{U}\omega \right\rangle &= \langle\lambda\omega|\lambda\omega\rangle \\ &= \lambda\lambda^* \langle\omega|\omega\rangle \\ &= |\lambda|^2 \end{aligned} \tag{72}$$

Hence $|\lambda|^2 = 1$

12 Generator in classical mechanics

Recall the lagrangian formalism:

$$\begin{gathered} \mathcal{L} = T - U = \frac{1}{2} m\dot{x} - U(x) \\ \frac{\partial \mathcal{L}}{\partial x} = \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}} \end{gathered} \tag{73}$$

The following equalities are trivial:

$$\begin{gathered} \frac{\partial \mathcal{L}}{\partial x} = \frac{\mathrm{d}}{\mathrm{d}t} p \\ \frac{\partial \mathcal{L}}{\partial p} = \frac{\partial}{\partial t} x \\ \frac{\partial \mathcal{L}}{\partial t} = -\frac{\mathrm{d}}{\mathrm{d}t} E \\ \frac{\partial \mathcal{L}}{\partial \theta} = -\frac{\mathrm{d}}{\mathrm{d}t} L \end{gathered} \tag{74}$$

Take a second to meditate on the above equalities, and we can find the following interpretation intuitive:

The time evolution of momentum results in a change in position in our "classical state" Lagrangian;

the time evolution of position results in a change in momentum;

the time evolution of energy results in a change in time;

and the time evolution of angular momentum results in a change in angle.

There is a special name for the above: the **generator** of the transformation. For example, momentum is the genrator of spatial change, position is the genertor of momentum change.

13 Schodinger's equation

13.1) Time evolution Operator: $\hat{U}(t)$

We have been representing our quantum state as $|\psi\rangle$. Now let's consider the time evolution via the **time evolution operator** $\hat{U}(t)$. It is defined as follows:

$$\hat{U}(t)|\psi\rangle = |\psi(t)\rangle \tag{75}$$

We observe several properties of this time evolution operator:

1. $\hat{U}(0)$ represents the time evolution after time zero. Obviously there's no change in our quantum state during 0 seconds, so

$$\hat{U}(0) = \hat{I} \tag{76}$$

2. Time evolution is reversible, so the linear operator $\hat{U}(t)$ is invertable.
3. Recall that the ineer product operation examines the probability of a system being at a quantum state. This probability is conserved over time (why? hypothesis?), so

$$\left\langle \hat{U}(t)\psi \middle| \hat{U}(t)\psi \right\rangle = \langle\psi|\psi\rangle = 1 \tag{77}$$

4. $\hat{U}(t)$ is an unitary operator. We try to proof this property in the following section

13.2) Proof of unitary operator $\hat{U}$

Given (writing $\hat{U}(t)$ as $\hat{U}$):

$$\left\langle \hat{U}\psi \middle| \hat{U}\psi \right\rangle = \langle\psi|\psi\rangle \tag{78}$$

$$\begin{aligned} \text{LHS} &= \left\langle \psi \middle| \hat{U}^\dagger\ \hat{U}\ \psi \right\rangle = \langle\psi|\ \hat{U}^\dagger\hat{U}|\psi\rangle \\ \text{RHS} &= \langle\psi|\psi\rangle = \langle\psi|\hat{I}|\psi\rangle \\ &\Rightarrow \langle\psi|\hat{U}^\dagger\hat{U}|\psi\rangle - \langle\psi|\hat{I}|\psi\rangle = 0 \\ &\langle\psi|\underbrace{\left(\hat{U}^\dagger\hat{U} - \hat{I}\right)}_{\text{investigate}}|\psi\rangle = 0 \end{aligned} \tag{79}$$

Let's investigate $\left(\hat{U}^\dagger\hat{U} - \hat{I}\right)$ by considering

$$\left(\hat{U}^\dagger\hat{U} - \hat{I}\right)^\dagger = \left(\hat{U}^\dagger\hat{U}\right)^\dagger - \hat{I}^\dagger = \hat{U}^\dagger\hat{U} - \hat{I} \tag{80}$$

Let $\hat{U}^\dagger\hat{U} - \hat{I} \equiv \hat{A}$, and denote its eigenbasis as $\{|a_i\rangle\}$. Plugging into Equation 79:

$$\langle\psi|\hat{A}|\psi\rangle = 0 \tag{81}$$

Since it is true for any state $|\psi\rangle$, we can subsitute $|\psi\rangle$ as $|a_i\rangle$, the eigenbasis of $\hat{A}$:

$$\begin{aligned} \langle a_i|\hat{A}|a_i\rangle &= 0 \\ \langle a_i|\lambda_i|a_i\rangle &= 0 \\ \lambda_i = 0 &\quad \text{for all } i \end{aligned} \tag{82}$$

Consider now:

$$
\begin{aligned}
\hat{A}|\psi\rangle &= \hat{A}\sum c_i|a_i\rangle \\
&= \sum \hat{A}c_i\widehat{a_i} \\
&= \sum \lambda_i c_i|a_i\rangle \\
&= 0
\end{aligned}
\tag{83}
$$

It is safe to conclude that $\hat{A} = \hat{0}$. Recalling that

$$
\begin{aligned}
\hat{A} = \hat{U}^\dagger\hat{U} - \hat{I} = 0 \\
\hat{U}^\dagger\hat{U} = \hat{I} \\
\hat{U}^\dagger = \hat{U}^{-1}
\end{aligned}
\tag{84}
$$

we have shown that $\hat{U}$ is an unitary operator. ■

13.3) Explicit time evolution

Consider a quantum state $|\psi\rangle$ that evolves over an infinitisemal time $\mathrm{d}t$. Summoning our friend Taylor, we can show

$$
\begin{aligned}
\hat{U}(\mathrm{d}t) &= \hat{U}(0) + \dot{\hat{U}}(0)\,\mathrm{d}t + \hat{\mathcal{O}}(\mathrm{d}t^2) \\
&= \hat{I} + \dot{\hat{U}}(0)\,\mathrm{d}t + \hat{\mathcal{O}}(\mathrm{d}t^2)
\end{aligned}
\tag{85}
$$

Now let's look at this infinitisemal time evolution operator acting on $|\psi\rangle$

$$
\begin{aligned}
\hat{U}(\mathrm{d}t)|\psi\rangle &= \hat{I}|\psi\rangle + \dot{\hat{U}}(0)\,\mathrm{d}t|\psi\rangle + \hat{\mathcal{O}}(\mathrm{d}t^2)|\psi\rangle \\
&= |\psi(\mathrm{d}t)\rangle = |\psi\rangle + \dot{\hat{U}}(0)\,\mathrm{d}t|\psi\rangle + \hat{\mathcal{O}}(\mathrm{d}t^2)|\psi\rangle
\end{aligned}
\tag{86}
$$

division of $\mathrm{d}t$ on both sides

$$
\frac{|\psi(\mathrm{d}t)\rangle - |\psi\rangle}{\mathrm{d}t} = \dot{\hat{U}}(0)|\psi\rangle + \underbrace{\frac{\hat{O}(\mathrm{d}t^2)|\psi\rangle}{\mathrm{d}t}}_{\text{negligible}}
\tag{87}
$$

as $\mathrm{d}t \to 0$:

$$
\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \dot{\hat{U}}(0)|\psi\rangle
\tag{88}
$$

Recalling $\hat{U}$ is unitary: $\hat{I} = \hat{U}^\dagger(\mathrm{d}t)\hat{U}(\mathrm{d}t)$, plugging into Equation 86 :

$$
\begin{aligned}
\hat{I} &= \left(\hat{I} + \dot{\hat{U}}(0)\,\mathrm{d}t + \hat{\mathcal{O}}(\mathrm{d}t^2)^\dagger\right)\left(\hat{I} + \dot{\hat{U}}(0)\,\mathrm{d}t + \hat{\mathcal{O}}(\mathrm{d}t^2)\right) \\
&= \hat{I} + \dot{\hat{U}}^\dagger(0)\,\mathrm{d}t + \dot{\hat{U}}(0)\,\mathrm{d}t + \hat{\mathcal{O}}(\mathrm{d}t^2))
\end{aligned}
\tag{89}
$$

as $\mathrm{d}t \to 0$,

$$
\begin{aligned}
\Rightarrow \dot{\hat{U}}^\dagger(0) + \dot{\hat{U}}(0) = 0 \\
\dot{\hat{U}}^\dagger(0) = -\dot{\hat{U}}(0)
\end{aligned}
\tag{90}
$$

$\dot{\hat{U}}$ is anti-hermitian.

Now consider

$$
\left(i\dot{\hat{U}}(0)\right)^\dagger = \dot{\hat{U}}^\dagger(0)i^\dagger = i\dot{\hat{U}}(0),
\tag{91}
$$

$i\dot{\hat{U}}(0)$ is Hermitian. Let $\widehat{H} = i\dot{\hat{U}}(0) \Rightarrow \dot{\hat{U}}(0) = \widehat{H}/i$

Now plugging back to Equation 88:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle &= \frac{\widehat{H}}{i}|\psi\rangle \\ i\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle &= \widehat{H}|\psi\rangle \end{aligned} \tag{92}$$

Recall that in classical mechanics, the generator of time evolution is Energy. We make an educated guess that $\widehat{H}$ is an energy operator. Then to align units on both sides, we multiply by $\hbar$ who is of the unit $[J \cdot s]$:

$$\boxed{i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \widehat{H}|\psi\rangle} \tag{93}$$

We have thus arrived at the time-dependent Schrodinger's equation. ∎

14 Generator of Momentum, Position and Energy

14.1) Momentum Operator

Recall that we proposed an energy operator $\widehat{H}$ on our way in deriving the Schrodinger's equation. This is actually the Hamiltonian of the system, and what we have shown is another way of getting the Hamiltonian– different than what we've done using Legendre Transform in Classical Mechanics.

The explicit formula of the Hamiltonian is

$$\widehat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{94}$$

Where $\hat{p}$ is the momentum operator, as we shall discuss below by taking a detour to the Translation Operator $\hat{T}(a)$

14.2) Translation Operator → Momentum Operator

We define the Translation Operator as a linear operator s.t. for any state vector $|x\rangle$ and any translational parameter a :

$$\hat{T}(a)|x\rangle = |x + a\rangle \tag{95}$$

For a quantum state on a continuous basis,

$$\hat{T}(a)|\psi\rangle = \hat{T}(a)\int \mathrm{d}x\psi(x)|x\rangle = \int \mathrm{d}x\psi(x)|x + a\rangle \tag{96}$$

$\hat{T}(a)$ is a translation that shifts all the quantum states by a.

It is self-evident that such a translation would preserve the overall probability of measurement

$$\left\langle \hat{T}\psi \middle| \hat{T}\psi \right\rangle = \langle\psi|\psi\rangle = 1 \tag{97}$$

It is not hard to proof that the translation operator is unitary. (Similar to the proof of time evolution operator $\widehat{U}$)

$$\hat{T}^\dagger = \hat{T}^{-1} \tag{98}$$

Now consider a small spacial translation $\mathrm{d}x$, and summoning our friend Taylor:

$$\hat{T}(\mathrm{d}x)|x\rangle = \hat{I} + \dot{\hat{T}}(0)\,\mathrm{d}x + \hat{\mathcal{O}}(\mathrm{d}x^2)|x\rangle \tag{99}$$

Division by $\mathrm{d}x$, and taking its limit to 0, we have:

$$\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle = \dot{\hat{T}}(0)|x\rangle \tag{100}$$

Recalling the Unitary property of $\hat{T}$, and reapeating the same step as we did in Equation 90, we can show that $\dot{\hat{T}}(0)$ is anti-hermitian.

To further exploit Equation 100, we use the anti-hermitian property to consider

$$\begin{gathered}\left(i\dot{\hat{T}}(0)\right)^\dagger = i\dot{\hat{T}}(0) \equiv= \hat{p} \\ \dot{\hat{T}}(0) = \hat{p}/i\end{gathered} \tag{101}$$

Equation 100 then becomes

$$i\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle = \hat{p}|x\rangle \tag{102}$$

Via observation, we can see that it is suggesting a generator of spatial translation. Our classical mechanics intuition tells us that this generator is the momentum operator. Now, unifying the units on both sides, we multiply by $\hbar$ to arrive at

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle = \hat{p}|x\rangle \tag{103}$$

It is known as the momentum operator in the position basis.

Repeating similar processes for the position operator and the angular momentum operator, we can collect the following series of equations:

$$\begin{cases} i\hbar\frac{\mathrm{d}}{\mathrm{d}p}|p\rangle = -\hat{x}|p\rangle \\ i\hbar\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle = \quad \hat{p}|x\rangle \\ i\hbar\frac{\mathrm{d}}{\mathrm{d}\theta}|\theta\rangle = \quad \hat{L}|\theta\rangle \\ i\hbar\frac{\mathrm{d}}{\mathrm{d}\psi}|t\rangle = \quad \widehat{H}|\psi\rangle \end{cases} \tag{104}$$

Where position $\hat{x}$ is the mementum generator, momentum $\hat{p}$ is the translational generator, angular momentum $\hat{L}$ is the anglular translation generator, and energy $\widehat{H}$ is the time-evolution generator.

This set of equations tells us, that physical observables can be understood as generators of some change in the quantum state.

More on the momentum operator $\hat{p}$

Consider

$$
\begin{aligned}
\hat{p}|\psi\rangle &= \hat{p}\int_{-\infty}^{\infty}\psi(x)|x\rangle\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\psi(x)\hat{p}|x\rangle\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty}\mathrm{d}x\psi(x)i\hbar\frac{\mathrm{d}}{\mathrm{d}x}|x\rangle \\
&= [i\hbar\psi(x)|x\rangle]|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\mathrm{d}x(i\hbar)\frac{\mathrm{d}\psi}{\mathrm{d}x}|x\rangle
\end{aligned}
\tag{105}
$$

We can see that the first term is zero, as our wavefunction be **localized** in space, which by definition means the wavefunction vanishes at infinity. Thus Equation 105 becomes

$$
\hat{p}|\psi\rangle = \int\mathrm{d}x\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x)\right)|x\rangle \tag{106}
$$

i.e. $\hat{p}$ can be seen as an operator s.t.

$$
|\psi\rangle \overset{\hat{p}}{\Longrightarrow} -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) \tag{107}
$$

This is equivalent to taking the ineer product of $\hat{p}$ and $|\psi\rangle$ in the position basis.

$$
\langle x|\hat{p}\psi\rangle = -i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\psi(x) \tag{108}
$$

15 Position-basis, momentum-basis, and Energy-basis Schrodinger's equations

Recall the time-dependent Schrodinger's equation, and the Hamiltonian operator on a system

$$
\begin{cases}
i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \hat{H}|\psi\rangle \\
\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})
\end{cases}
\tag{109}
$$

$$
\Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \frac{\hat{p}^2}{2m}|\psi\rangle + V(\hat{x})|\psi\rangle \tag{110}
$$

Taking the inner product on the position basis...

$$
\begin{aligned}
\langle x|i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle &= \langle x|\frac{\hat{p}^2}{2m}|\psi\rangle + \langle x|V(\hat{x})|\psi\rangle \\
i\hbar\frac{\partial}{\partial t}\langle x|\psi\rangle &= -\frac{\hbar^2}{2m}\frac{\partial^2}{(\partial x)^2}\langle x|\psi\rangle + V(x)\langle x|\psi\rangle
\end{aligned}
\tag{111}
$$

Recognizing that $\langle x|\psi\rangle$ represents coefficient of the quantum state $|\psi\rangle$in the position basis $|x\rangle$, this is the wavefunction $\psi(x,t)$ The above then simplifies to

$$
\boxed{i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x,t)} \tag{112}
$$

And this is the Schrodinger's equation in the position basis.

Similarly, taking the inner product of Equation 110 on the momentum basis, and given that $\langle p|\hat{x}|\psi\rangle = i\hbar\frac{\mathrm{d}}{\mathrm{d}p}\varphi(p)$, where $\varphi(p)$ is the momentum wavefunction, we can show

$$i\hbar\langle p|\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \langle p|\frac{\hat{p}^2}{2m}|\psi\rangle + \langle p|V(\hat{x})|\psi\rangle \tag{113}$$

$$\boxed{\Rightarrow \quad i\hbar\frac{\partial}{\partial t}\varphi(p,t) = \frac{p^2}{2m}\varphi(p,t) + V\left(i\hbar\frac{\partial}{\partial p}\right)\varphi(p,t)} \tag{114}$$

This is the Schrodinger's equation in the momentum basis.

Taking the inner product of the time-dependent schrodinger's equation with respect to the energy basis,

$$i\hbar\langle E_i|\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle = \langle E_i|\widehat{H}|\psi\rangle \tag{115}$$

$$\boxed{\Rightarrow i\hbar\frac{\mathrm{d}}{\mathrm{d}t}c_{i(t)} = E_i c_{i(t)}} \tag{116}$$

where $c_i$represents the coefficients of the quantum state $|\psi\rangle$ in the energy basis $|E_i\rangle$, and E_i is the energy eigenvalue. This is the Schrodinger's equation in the energy basis.