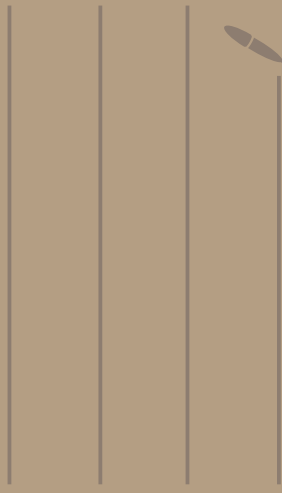


Quantum Mechanics 2020

PHYS - C0252

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26.10.2020 Lecture I

ILO 3

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

Hilbert space

- Complete inner product space

1. $\mathcal{H} = \{|\psi\rangle\}$ is a vector space over a scalar field \mathbb{C}

2. There is a scalar product defined on \mathcal{H} s.t. $\forall |\phi\rangle, |\psi\rangle \in \mathcal{H}$ we have

$$\langle \psi | \psi \rangle = (|\psi\rangle, |\psi\rangle) \in \mathbb{C} \quad \text{s.t.}$$

$$(a) \langle \psi | \phi \rangle = (\langle \phi | \psi \rangle)^* = \langle \phi | \psi \rangle^*$$

$$(b) \langle \psi | a\phi_1 + b\phi_2 \rangle = \langle \psi | (a|\phi_1\rangle + b|\phi_2\rangle) \\ = a\langle \psi | \phi_1 \rangle + b\langle \psi | \phi_2 \rangle$$

$$(c) \langle \psi | \psi \rangle \geq 0; \langle \psi | \psi \rangle = 0 \iff |\psi\rangle = 0$$

Physical states are those elements of \mathcal{H} for which norm is unity, i.e., $\langle \psi | \psi \rangle = 1$

Math recap on vector space

A vector space V over a scalar F is a set where $+$ is defined

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

$$1. u + (v + w) = (u + v) + w$$

$$2. u + v = v + u$$

$$3. \exists 0 \in V \text{ s.t. } u + 0 = u$$

$$4. \forall v \in V \exists -v \in V \text{ s.t. } v + (-v) = 0$$

$$5. a(bv) = (ab)v$$

$$6. 1v = v, \text{ where } 1 \in F$$

$$7. a(u + v) = au + av$$

$$8. (a + b)v = av + bv$$

\Rightarrow we can define a norm $\| \psi \| = \sqrt{\langle \psi | \psi \rangle} = \| |\psi\rangle \| \geq 0$

$$\text{ex. } \cdot |\langle \psi | \phi \rangle| \leq \| \psi \| \| \phi \| \quad \text{Cauchy-Schwarz inequality}$$

$$\text{ex. } \cdot \| a|\psi\rangle + |\phi\rangle \| \leq \| a|\psi\rangle \| + \| |\phi\rangle \| \quad \text{triangle inequality}$$

3. All Cauchy sequences converge into \mathcal{H} .

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

\rightarrow not going to ask about this in the exam

Bra and ket vectors

- We define the ket vectors as elements of \mathcal{H} , i.e., $\mathcal{H} = \{|\psi\rangle\}$

- We define a bra vector $\langle\phi|$ through the inner product s.t.

$$\langle\phi|\psi\rangle = (\langle\phi|, |\psi\rangle) \in \mathbb{C}$$

- observation: we can identify each bra vector $\langle\phi|$ with a linear and bounded functional $f_\phi \in \mathcal{L}$

\Rightarrow Riesz representation theorem
• not gonna use about this in exam
tells that for each $f_\phi \exists |\phi\rangle \in \mathcal{H}$

\Rightarrow There is a one-to-one correspondence between $\mathcal{H} \in \{|\psi\rangle\}$ and $\mathcal{H}^* \in \{\langle\phi|\}$

Math.

- A functional f acting on space A is a mapping $f: A \rightarrow \mathbb{C}$

Linear operator

• \hat{A} is a linear oper. on \mathcal{H}

$\Leftrightarrow \hat{A}: \mathcal{H} \rightarrow \mathcal{H}$ st. $\forall |\psi\rangle, |\phi\rangle \in \mathcal{H}, a, b \in \mathbb{C}$

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

• We also define notation as

$$\hat{A}|\psi\rangle \equiv A|\psi\rangle \equiv |\hat{A}\psi\rangle$$

space of linear operators on \mathcal{H}

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

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

Eigenvalues and eigenstates

• Eigen state $|\psi_a\rangle \in \mathcal{H}$ related to the eigenvalue $\lambda \in \mathbb{C}$ of operator $\hat{A} \in \mathcal{L}(\mathcal{H})$

satisfies
$$\hat{A}|\psi_a\rangle = \lambda|\psi_a\rangle$$

28.10.2020 Lecture II

L.O.S

1. Use bases to represent operators
2. Identify the minimal mathematical structure to describe a physical system quantum mechanically
3. Differentiate between a measurement outcome and its expectation value ← moved to lecture 3

Outer Product

We define the outer product $|\psi\rangle\langle\phi| : \mathcal{H} \rightarrow \mathcal{H}$, where $|\psi\rangle, |\phi\rangle \in \mathcal{H}$

s.t. $\forall |\chi\rangle \in \mathcal{H}$ we have

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

Bases of \mathcal{H}

- a set $\{|\phi_i\rangle\}_{i=1}^N \subset \mathcal{H}$ is called linearly independent if $\sum_{i=1}^N c_i |\phi_i\rangle = 0$ where $c_i \in \mathbb{C}$, $N \in \mathbb{Z}_+$, then $c_i = 0 \forall i$
- $\dim\{\mathcal{H}\}$ is the largest N for which such a linearly independent set of vectors exists
- The set is called complete if $\forall |\psi\rangle \in \mathcal{H}$ $\exists c_k \in \mathbb{C}$ s.t. $|\psi\rangle = \sum_{k=1}^N c_k |\phi_k\rangle$
(Similarly for infinite-dimensional spaces)
- A complete set of linearly independent vectors $\{|\phi_k\rangle\}$ is a basis of \mathcal{H}

• for orthonormal basis, $\{|\phi_k\rangle\}$ we have

$$\langle\phi_l|\phi_m\rangle = \delta_{lm} = \begin{cases} 0, & l \neq m \\ 1, & l = m \end{cases}$$

• Ob. for verification for orthonormal basis $\{|\phi_k\rangle\}$:

take an arbitrary $|\psi\rangle \in \mathcal{H}$.

we have $|\psi\rangle = \sum_k c_k |\phi_k\rangle$

$\Downarrow \langle \phi_m |$

$$\langle \phi_m | \psi \rangle = \sum_k c_k \langle \phi_m | \phi_k \rangle = c_m$$

Thus $|\psi\rangle = \sum_m \langle \phi_m | \psi \rangle |\phi_m\rangle$

$$= \sum_m |\phi_m\rangle \langle \phi_m | \psi \rangle$$

$$= \left(\sum_m |\phi_m\rangle \langle \phi_m | \right) |\psi\rangle$$

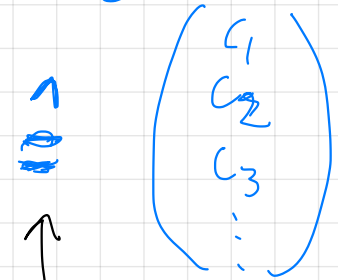
$\underbrace{\hspace{10em}}_{=: \hat{I}}$

states v.s. vectors

• fix an orthonormal basis $\{|\phi_k\rangle\}$

and a $|\psi\rangle \in \mathcal{H}$

$$|\psi\rangle = \sum_k c_k |\phi_k\rangle$$



represented by cish

Operations V.S. Matrices

Let $\hat{A} \in \mathcal{L}(\mathcal{V})$ and $\{|\phi_m\rangle\}$ an orthonormal basis

$$\tilde{A} = \tilde{I} \hat{A} \tilde{I} = \left(\sum_m |\phi_m\rangle\langle\phi_m| \right) \hat{A} \left(\sum_k |\phi_k\rangle\langle\phi_k| \right)$$

$$= \sum_{m,k} |\phi_m\rangle\langle\phi_m| \hat{A} |\phi_k\rangle\langle\phi_k|$$

$A_{mk} \in \mathbb{C}$

$$= \sum_{m,k} A_{mk} |\phi_m\rangle\langle\phi_k|$$

$$\approx \begin{pmatrix} A_{11} & A_{12} & \dots & \dots \\ A_{21} & A_{22} & \dots & \dots \\ A_{31} & \dots & \dots & \dots \\ \vdots & \dots & \dots & \dots \end{pmatrix}$$

operation

$$\hat{A} |\psi\rangle = \sum_{m,k} A_{mk} |\phi_m\rangle\langle\phi_k| \sum_l c_l |\phi_l\rangle$$

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

$$\langle\phi_m| \hat{A} |\psi\rangle = \sum_k A_{mk} c_k$$

$m-1$ zeroes

$$= \begin{pmatrix} 0 & 0 & \dots & 1 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

math on complex components

$\forall z \in \mathbb{C}$ we have $x, y \in \mathbb{R}$

$$z = x + iy, \quad i \text{ is imaginary}$$

$$z^* = x - iy$$

Adjoint

Fix $\hat{A} \in \mathcal{L}(\mathcal{H})$. We def: $\hat{A}^*: \mathcal{H} \rightarrow \mathcal{H}$
s.t. $\langle \hat{A}^* \psi, \phi \rangle = \langle \psi, \hat{A} \phi \rangle$

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

We observe that the operation

$\langle \phi | \hat{A}$ is a linear functional on \mathcal{H} and is bounded since \hat{A} is bounded.

Thus it follows from Riesz representation theorem that $\exists |\phi'\rangle \in \mathcal{H}$ s.t.

$$\langle \phi' | = \langle \phi | \hat{A}$$

This defines also a linear operator

$$\hat{A}^* | \phi \rangle = | \phi' \rangle$$

\uparrow
adjoint of \hat{A}

ex. $\langle \phi | c | \psi \rangle = (| \phi \rangle, c | \psi \rangle)$
 $= c (| \phi \rangle, | \psi \rangle)$
 $= (c^* | \phi \rangle, | \psi \rangle)$

$$\Rightarrow c^\dagger = c^* \text{ } \leftarrow \text{ } \hat{c}$$

Properties of adjoint

$$(\hat{A}^\dagger)^\dagger = \hat{A} \quad (\text{not proved here})$$

$$(c \hat{A})^\dagger = c^* \hat{A}^\dagger$$

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

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

About notation

$$\langle \phi | \hat{A} | \psi \rangle = (| \phi \rangle, \hat{A} | \psi \rangle) = (\hat{A}^* | \phi \rangle, | \psi \rangle)$$

$$= \langle \hat{A}^* \phi | \psi \rangle \quad \leftarrow \text{sometimes denoted like this}$$

Hermitian operators

- $\hat{A} \in \mathcal{L}(\mathcal{H})$ is defined Hermitian iff $\hat{A}^\dagger = \hat{A}$

- These (generalized) spectral theorem that states that

$\forall \hat{A}^\dagger = \hat{A} \in \mathcal{L}(\mathcal{H}) \exists \{|\psi_k\rangle\} \subset \mathcal{H}$
which is a complete ^(orthonormal) basis of \mathcal{H}
and $\{\lambda_k\} \subset \mathbb{R}$ s.t.

$$\hat{A}|\psi_k\rangle = \lambda_k|\psi_k\rangle$$

- Thus we can express $\hat{A} = \sum_k \lambda_k |\psi_k\rangle\langle\psi_k|$

Postulates of quantum mechanics

- I) For each physical system there exists a corresponding (Hilbert) space
- II) Each physical state of this system can be represented by a quantum state $|\psi\rangle \in \mathcal{H}$, where $\langle \psi | \psi \rangle = 1$ (in case of partial description of the full system, or subsystem may be described by a so-called density operator)
- III) For each measurable quantity of the system A we have $\hat{A} \in \mathcal{L}(\mathcal{H})$ s.t. $\hat{A}^\dagger = \hat{A}$
- In an ideal measurement any measurement outcome equals to an eigenvalue of \hat{A}

Measurement

- Let $|\psi\rangle \in \mathcal{H}$
- Let $\hat{A}^\dagger = \hat{A} \in \mathcal{L}(\mathcal{H})$ with a ^{discrete} spectrum $\{a_n\}_n$ and the corresponding eigenstates $\{|\phi_{n,i}\rangle\}_{n,i=1}^{g_n}$, where g_n equals the amount of degeneracy.
Thus $\hat{A}|\phi_{n,i}\rangle = a_n|\phi_{n,i}\rangle$.
- Let $\{|\phi_{n,i}\rangle\}$ orthonormal complete basis of \mathcal{H}
- The probability of obtaining a measurement result a_n is given by $P(a_n) \equiv \sum_{i=1}^{g_n} |\langle \phi_{n,i} | \psi \rangle|^2$

After measurement

If we measure an \hat{A} for $|\psi\rangle \in \mathcal{H}$ (all definitions as above),
the state of the system collapses into

$$|\psi'\rangle = \frac{\hat{P}_h |\psi\rangle}{\|\hat{P}_h |\psi\rangle\|}, \quad \hat{P}_h = \sum_{i=1}^{g_h} |\phi_{h,i}\rangle \langle \phi_{h,i}|$$

Def
 $\hat{P} \in \mathcal{L}(\mathcal{H})$ is a projector iff $\hat{P}^2 = \hat{P}$

→ this is a projector into the subspace corresponding to the subspace spanned by the eigenstates $\{|\phi_{h,i}\rangle\}_{i=1}^{g_h}$

Temporal evolution

Let $|\psi\rangle \in \mathcal{H}$ and $\hat{H} \in \mathcal{L}(\mathcal{H})$ s.t. \hat{H} is classical Hamiltonian which is typically equal to the total energy of the system in question. Thus we have

$$i\hbar \partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \leftarrow \text{Schrödinger equation}$$

• Note that \hat{H} may depend on time through temporarily dependent parameters $\{\alpha_k(t)\}$. That is $\hat{H} = \hat{H}[\alpha_1(t), \dots]$

2.11.2020 Lecture III

LLOs

1. Distribute between measurement outcome and its expectation value
2. Identify continuous bases for Hilbert spaces
3. Apply Lagrangian formalism to quantize physical systems

Expectation values

• Let $\hat{A} \in \mathcal{L}(\mathcal{H})$ and $|\psi\rangle \in \mathcal{H}$

• We define the expectation value of \hat{A} in the state $|\psi\rangle$ is defined by

$$\langle A \rangle \equiv \langle \psi | \hat{A} | \psi \rangle, \quad \langle \hat{A} \rangle \equiv \langle \psi | \hat{A} | \psi \rangle$$

• Let A be an observable $\Rightarrow \hat{A} = \hat{A}^\dagger$

$\Rightarrow \exists \{|\phi_k\rangle\}$ s.t. $\langle \phi_k | \phi_m \rangle = \delta_{km}$

and $\hat{A}|\phi_k\rangle = a_k|\phi_k\rangle, \quad a_k \in \mathbb{R}$

$$\Rightarrow |\psi\rangle = \sum_k c_k |\phi_k\rangle$$

$$\langle \psi | \hat{A} | \psi \rangle = \left(\sum_k c_k \langle \phi_k | \right)^\dagger \hat{A} \sum_l c_l |\phi_l\rangle$$

$$= \left(\sum_m c_m \langle \phi_m | \right)^\dagger \sum_k c_k a_k |\phi_k\rangle$$

$$= \sum_{m,k} c_m^* c_k a_k \langle \phi_m | \phi_k \rangle$$

$$= \sum_k a_k |c_k|^2 = \sum_k a_k P(a_k)$$

$\underbrace{\hspace{10em}}_{P(a_k)}$

Variance

• We define the variance of \hat{A} in $|\psi\rangle$

$$\Delta A^2 \equiv \langle \psi | (\hat{A} - \langle \psi | \hat{A} | \psi \rangle)^2 | \psi \rangle$$

$$= \langle \psi | \hat{A}^2 | \psi \rangle - (\langle \psi | \hat{A} | \psi \rangle)^2$$

$$= \sum_k a_k^2 P_k - \left(\sum_k a_k P_k \right)^2$$

Continuous bases

- Continuous bases are sometimes required, for example if continuous variables are used.
- Let $\{|\psi_\alpha\rangle\}$ where $\alpha \in \mathbb{R}$ s.t.

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

- Note that $\langle \psi_\alpha | \psi_\alpha \rangle = \delta(0) = \infty$
thus $|\psi_\alpha\rangle$ is not normalizable.

\Rightarrow we work with Rigged Hilbert space that allows these \leftarrow maybe more on this later

- In any case, we can use these as

$$|\psi\rangle = \int c_\alpha |\psi_\alpha\rangle d\alpha = \int \langle \psi_\alpha | \psi \rangle |\psi_\alpha\rangle d\alpha$$

$$c_\alpha = \langle \psi_\alpha | \psi \rangle = \psi(\alpha) \leftarrow \text{wave function}$$

$$= \int |\psi_\alpha\rangle \langle \psi_\alpha | \psi \rangle d\alpha = \left(\int |\psi_\alpha\rangle \langle \psi_\alpha| d\alpha \right) |\psi\rangle, \quad \forall |\psi\rangle \in \mathcal{H}$$

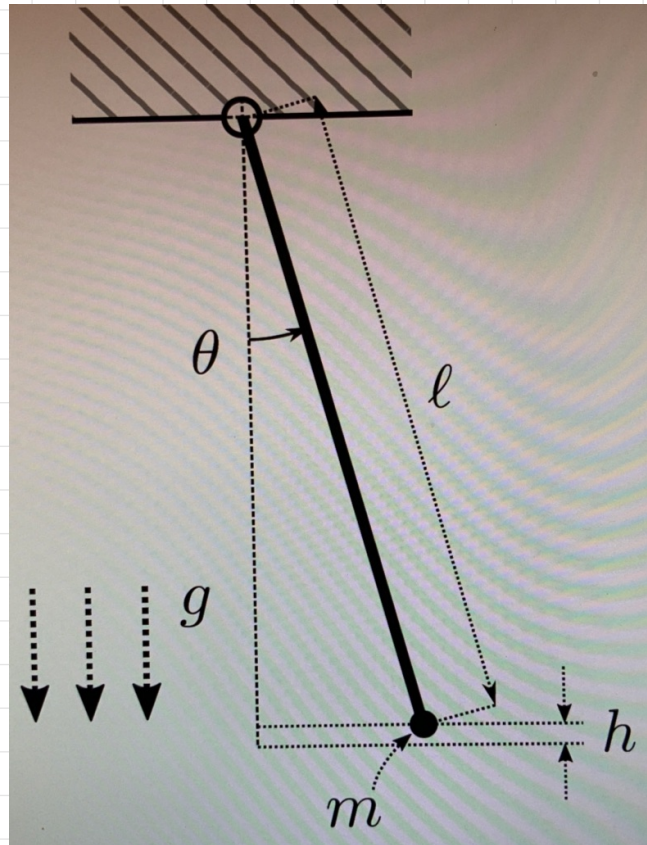
- Measurement probability of the measurement outcome $[\alpha, \alpha + d\alpha]$ is described by

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

math $f \in C^\infty$

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

Quantization of quantum systems:
classical pendulum



• Pick our generalized position to be

$$q = l\theta$$

• The potential energy is described by q (not \dot{q}). Thus it assumes the form

$$V = mgh = mgl(1 - \cos\theta) \approx \frac{1}{2} mgl\theta^2 = \frac{mg}{2l} q^2$$

• The kinetic energy

is described by \dot{q} . Thus we have

$$T = \frac{1}{2} m v^2 = \frac{1}{2} m l^2 \dot{\theta}^2 = \frac{1}{2} m \dot{q}^2$$

• Lagrangian is defined as

$$L \equiv T - V = \frac{1}{2} m l^2 \dot{\theta}^2 - \frac{1}{2} mgl\theta^2 = \frac{1}{2} m \dot{q}^2 - \frac{mg}{2l} q^2$$

• Generalized momentum is defined as

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

← consider q and \dot{q} as independent variables here

Method Taylor series

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

• The Hamiltonian is defined as

$$H = \dot{q}p - L = m\dot{q}^2 - \left(\frac{1}{2} m \dot{q}^2 - \frac{mg}{2l} q^2 \right)$$

$$= \frac{p^2}{2m} + \frac{mg}{2l} q^2 = T + V$$

this is the Hamiltonian of 1D harmonic oscillator

• Quantization proceeds as follows:

1. operator substitution

$$q \rightarrow \hat{q}; \gamma_L \rightarrow \gamma_L, \quad \dot{q} = \dot{q}^{\text{cl}}$$

$$p \rightarrow \hat{p}; \gamma_L \rightarrow \gamma_L, \quad \dot{p} = \dot{p}^{\text{cl}}$$

2. $[\hat{p}, \hat{q}] \equiv \hat{p}\hat{q} - \hat{q}\hat{p} = -i\hbar$

3. $H \rightarrow \hat{H}$ with the help of 1.

[for above H we have $\hat{H} = \frac{\hat{p}^2}{2m} + \frac{mg}{2l} \hat{q}^2$]

4. $i\hbar \partial_t |\psi\rangle = \hat{H} |\psi\rangle$

Lecture 4

ILOS

1. Apply operator exponential to symbolically solve the Schrödinger eq.
2. Differentiate between a qubit and a general quantum system
3. Represent qubit state on the Bloch sphere

Unitary temporal evolution

Let $|\psi(t=0)\rangle \in \mathcal{H}$ and $\hat{H} \in \mathcal{L}(\mathcal{H})$ be the Hamiltonian. Schrödinger equation yields the temporal evolution as $\exists |\psi(t)\rangle \in \mathcal{H}$ s.t. $|\psi(t=0)\rangle = |\psi(0)\rangle$ and $i\hbar \partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \Leftrightarrow \partial_t |\psi(t)\rangle = -\frac{i\hat{H}}{\hbar} |\psi(t)\rangle$

- Note that we assumed that \hat{H} is independent of time

Let us define $e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!}$, for $\forall \hat{A} \in \mathcal{L}(\mathcal{H})$

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

Thus $|\psi(t)\rangle = \underbrace{e^{-i\hat{H}t/\hbar}}_{\equiv \hat{U}(t)} |\psi(0)\rangle$

Math $\partial_x f(x) = \lambda f(x) \Rightarrow f(x) = A e^{\lambda x} \left| \begin{matrix} e^x \\ e^x = 1 \end{matrix} \right.$

We observe that $\hat{U}(t)^\dagger \hat{U}(t) = e^{i\hat{H}t/\hbar} e^{-i\hat{H}t/\hbar} = \hat{U}^{-1} \hat{U} = \mathbb{I}$
 ex.

which means by definition the \hat{U} is unitary

Let $\{|\psi_m\rangle\} \subset \mathcal{H}$ be eigenbasis of \hat{H} , i.e., $\hat{H} |\psi_m\rangle = a_m |\psi_m\rangle$ where $\{a_m\} \in \mathbb{R}$

Thus we can expand $|\psi(0)\rangle = \sum_{n=0}^{\infty} c_n |\psi_n\rangle$, $c_n \in \mathbb{C}$

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

Case of time-dependent Hamiltonian

- Still the Schrödinger equation is about

$$i\partial_t |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$

and the evolution is unitary

(w/ $\hat{U}(t) \in \mathcal{L}(\mathcal{H})$ s.t.

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

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

$$\Rightarrow i\partial_t \hat{U}(t) = \hat{H}(t) \hat{U}(t)$$

is equivalent to Schrödinger eq.

ex.

build $\hat{U}(t)$ for $\hat{H}(t)$

Properties of unitary operators

$$\bullet (\hat{U}_1 \hat{U}_2)^\dagger = \hat{U}_2^\dagger \hat{U}_1^\dagger = \hat{U}_2^{-1} \hat{U}_1^{-1} = (\hat{U}_2 \hat{U}_1)^{-1}$$

$\Rightarrow \hat{U}_1 \hat{U}_2$ is also unitary

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

we define $|\psi'\rangle = \hat{U} |\psi\rangle$

$$|\phi'\rangle = \hat{U} |\phi\rangle$$

$$\langle \psi' | \phi' \rangle = \langle \psi | \hat{U}^\dagger \hat{U} | \phi \rangle = \langle \psi | \hat{U}^{-1} \hat{U} | \phi \rangle$$

$$= \langle \psi | \hat{U}^\dagger \hat{U} | \phi \rangle = \langle \hat{U}^{-1} \hat{U} | \psi \rangle, \hat{U} | \phi \rangle$$

$$= \langle \psi | \phi \rangle$$

- Unitary operators can be considered as rotations (sometimes reflections as well)

Qubit

• A qubit can refer either to a physical system or to a mathematical construction. In either case it is modeled by a two-level quantum system as follows;

• Let $\mathcal{H}_2 = \text{Span}\{|0\rangle, |1\rangle\}$, where $\langle 0|\hat{\sigma}_z|0\rangle = 1$ and $\langle 1|\hat{\sigma}_z|1\rangle = -1$

• \mathcal{H}_2 fully describes all possible states of the qubit where

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

• Thus the Hamiltonian \hat{H} has just two eigenvalues $E_1 \leq E_2$ and the corresponding eigenvectors are $|g\rangle$ and $|e\rangle$, respectively.

• Thus $\hat{H} = E_1 |g\rangle\langle g| + E_2 |e\rangle\langle e|$

$$= \frac{E}{2} (-|g\rangle\langle g| + |e\rangle\langle e|)$$

$$E = E_2 - E_1$$

$$+ \frac{(E_1 - E_2)}{2} |g\rangle\langle g| - \frac{(E_1 - E_2)}{2} |e\rangle\langle e|$$

Math Let $\{|\psi_m\rangle\} \subset \mathcal{H}$

$$\text{Span}(\{|\psi_m\rangle\}) = \left\{ \sum_m c_m |\psi_m\rangle \mid c_m \in \mathbb{C} \right\}$$

$$= \frac{E}{2} (-|g\rangle\langle g| + |e\rangle\langle e|) + \frac{E_1 - E_2}{2} \hat{I}$$

• Thus $\hat{H}_g = \frac{E}{2} (|g\rangle\langle g| - |e\rangle\langle e|)$ We can drop this since it just changes the phase of all $|\psi\rangle \in \mathcal{H}$

• We can define the qubit states $|0\rangle \equiv |g\rangle$

$$|1\rangle \equiv |e\rangle$$

• Thus $\hat{H}_g = -\frac{E}{2} \hat{\sigma}_z$, $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1|$

$$\hat{H}_g = \begin{pmatrix} -\frac{E}{2} & 0 \\ 0 & +\frac{E}{2} \end{pmatrix}$$

• The temporal evolution is given by

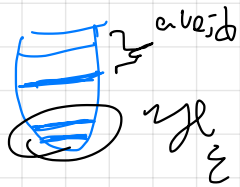
$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\psi(0)\rangle, \quad |\psi(0)\rangle = c_0|0\rangle + c_1|1\rangle$$

$$= e^{+i\frac{E}{2}\hat{\sigma}_z t/\hbar} |\psi(0)\rangle$$

$$= e^{i\frac{E}{2}t/\hbar} c_0|0\rangle + e^{-i\frac{E}{2}t/\hbar} c_1|1\rangle$$

How to get a qubit from a physical system

- Confine dynamics to the subspace of two states
- For example, a spin is a natural two-level system, but confined (for example in atoms)
- For example, non-linear system where $\epsilon_0 < \epsilon_1 < \epsilon_2 < \epsilon_3 \dots$ we exist values of $\hbar \omega$ s.t. $\epsilon_1 - \epsilon_0 \approx \epsilon_2 - \epsilon_1$.



Pauli operators

$$\begin{aligned} \text{Def. } \hat{\sigma}_z &= |0\rangle\langle 0| - |1\rangle\langle 1| \\ \hat{\sigma}_x &= |0\rangle\langle 1| + |1\rangle\langle 0| \\ \hat{\sigma}_y &= i|0\rangle\langle 1| - i|1\rangle\langle 0| \end{aligned}$$

Properties

$$\hat{\sigma}_\alpha^2 = I, \quad \hat{\sigma}_\alpha^\dagger = \hat{\sigma}_\alpha$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = \sum_{k \in \{x, y, z\}} \epsilon_{ijk} \hat{\sigma}_k, \quad i, j \in \{x, y, z\}$$

where $\epsilon_{ijk} = \begin{cases} 1, & \epsilon_{xyz} = \epsilon_{zyx} = \epsilon_{yxz} \\ -1, & \epsilon_{yxz} = \epsilon_{zxy} = \epsilon_{xzy} \\ 0, & \text{otherwise} \end{cases}$

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

ex. show $e^{i\vec{a} \cdot \hat{\sigma}} = I \cos \varrho + \vec{a} \cdot \hat{\sigma} \sin \varrho$

where $\|\vec{a}\| = 1$

$$\vec{a} \cdot \hat{\sigma} = a_x \hat{\sigma}_x + a_y \hat{\sigma}_y + a_z \hat{\sigma}_z$$

Bloch Sphere

Qubit state can always be expressed as

$$|\psi\rangle = \cos(\theta/2) |0\rangle + e^{i\phi} \sin(\theta/2) |1\rangle$$

↑ Polar angle
↑ azimuthal angle

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

$$\begin{aligned} \langle \psi | \hat{A} | \psi \rangle &= \langle \psi | \hat{A} e^{-i\alpha} e^{i\alpha} | \psi \rangle = \langle \psi | e^{-i\alpha} \hat{A} e^{i\alpha} | \psi \rangle \\ &= \langle e^{i\alpha} \psi | \hat{A} e^{i\alpha} | \psi \rangle, \end{aligned}$$

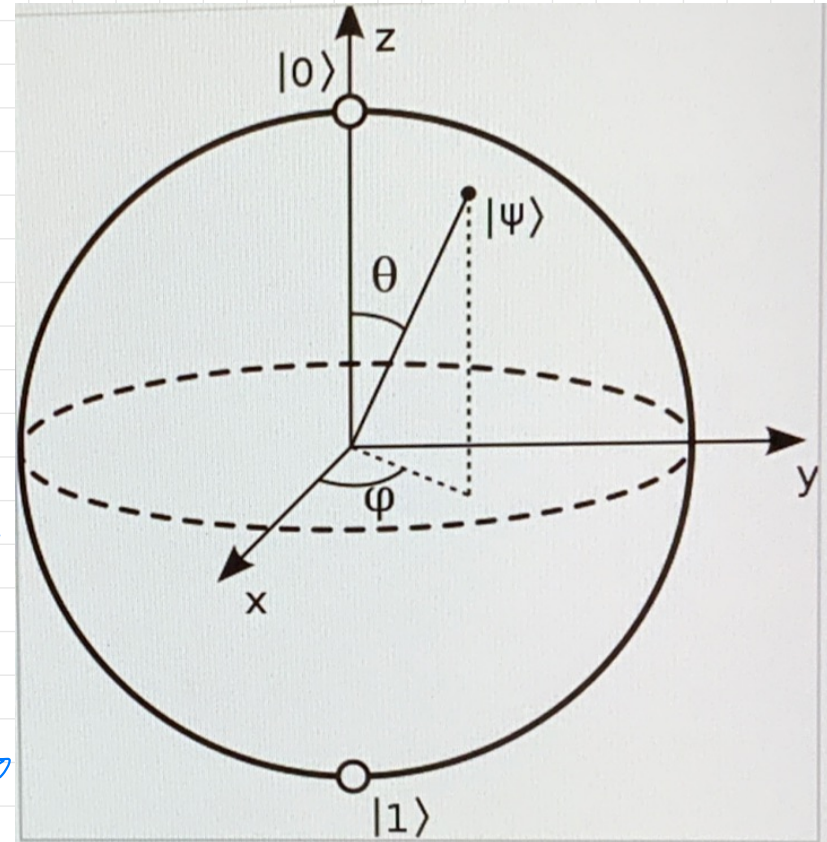
we can always choose $c_0 \in \mathbb{R}$ in $|\psi\rangle = c_0 |0\rangle + c_1 |1\rangle$

- Thus for each state there are unique

$\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$ which correspond

to a point on a unit sphere as shown here →

Bloch sphere representation



ex.

$\vec{U}(t)$ are rotations of
the Bloch vector

Lecture 5

QLOs

1. Apply tensor product to construct a quantum register of N qubits
2. Identify the constituents of a quantum algorithm
3. Apply the commutator to identify conserved quantities

Tunable Hamiltonian for quantum gates

Let span $\{|0\rangle, |1\rangle\} = \mathcal{H}_2$ and assume that control over the Hamiltonian s.t.

$$\hat{H} = E_0 \vec{a}(t) \cdot \vec{\sigma}, \text{ where } \vec{a} \in \mathbb{R}^3, \|\vec{a}\|=1$$

$E_0, \text{ angle} \in \mathbb{R}$

thus any unitary evolution $\hat{U} = \cos(\theta)\hat{I} + \vec{b} \cdot \vec{\sigma} \sin(\theta)$ (which is referred to as a single qubit gate) can be implemented, for example, by a control sequence

$$\vec{a}(t) = \begin{cases} 0, & t < 0 \\ E_0 \vec{b}, & 0 \leq t \leq 2\theta/\omega \\ 0, & t > 2\theta/\omega \end{cases}$$

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

$$\hat{H} = -\frac{\hbar}{2} \sum \hat{\sigma}_z \quad \text{and apply a sieve} \quad \hat{H}_{eff}(t) = \frac{\hbar}{2} \sin(\omega t + \phi)$$

- That will result in so-called Rabi oscillations to be discussed later

Single-qubit gates: examples

- The NOT gate corresponds to $\hat{\sigma}_x = |0\rangle\langle 1| + |1\rangle\langle 0| \stackrel{\text{matrix}}{=} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
- Hadamard gate corresponds to $\hat{H}_3 = \frac{\hat{\sigma}_z + \hat{\sigma}_x}{2} \stackrel{\text{matrix}}{=} \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \stackrel{\text{matrix}}{=} \hat{H}_3$
- Phase flip corresponds to $\hat{\sigma}_z = |0\rangle\langle 0| - |1\rangle\langle 1| \stackrel{\text{matrix}}{=} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \hat{\sigma}_z = \hat{Z}$

Edm

- Find $\hat{U}(t)$ implement these
- $\hat{H}_3 \hat{\sigma}_x \hat{H}_3 = \hat{\sigma}_z$
- $\hat{H}^\dagger = \hat{H} = \hat{H}^{-1}$

Qubit measurement

Let $|\psi\rangle \in \mathcal{H}_2$ be quantum state. thus $|\psi\rangle = c_0|0\rangle + c_1|1\rangle$, where $c_0, c_1 \in \mathbb{C}$ s.t. $|c_0|^2 + |c_1|^2 = 1$

• Thus

the measurement probabilities are given by

$$P_0 = |\langle 0 | \psi \rangle|^2 = |c_0|^2$$

$$P_1 = |\langle 1 | \psi \rangle|^2 = |c_1|^2 = 1 - |c_0|^2$$

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

$$P_0 = |\langle 0 | \hat{U} |\psi\rangle|^2 = \langle 0 | \hat{U}^\dagger |0\rangle \langle 0 | \hat{U} |\psi\rangle = |\langle \tilde{0} | \psi \rangle|^2, \text{ where } |\tilde{0}\rangle = \hat{U}^\dagger |0\rangle$$

similarly for $P_1 = |\langle 1 | \psi \rangle|^2 = |\langle \tilde{1} | \psi \rangle|^2$, where $|\tilde{1}\rangle = \hat{U}^\dagger |1\rangle$

2-qubit system

The Hilbert space $\mathcal{H}_4 = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)}$ is 4-dimensional

- Thus single-qubit operators are given by

$$\hat{A}_1 \otimes \hat{I} \quad \text{and} \quad \hat{I} \otimes \hat{A}_2, \quad \text{where } \hat{A}_1 \in \mathcal{L}(\mathcal{H}_2^{(1)}) \\ \hat{A}_2 \in \mathcal{L}(\mathcal{H}_2^{(2)})$$

- Let $\hat{A} \otimes \hat{B} = \hat{C} \in \mathcal{L}(\mathcal{H}_4)$
 $\hat{D} \otimes \hat{E} = \hat{F} \in \mathcal{L}(\mathcal{H}_4)$

$$\Rightarrow \hat{C}\hat{F} = (\hat{A} \otimes \hat{B})(\hat{D} \otimes \hat{E}) = (\hat{A}\hat{D}) \otimes (\hat{B}\hat{E})$$

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

$$\begin{aligned} |00\rangle &\equiv |0\rangle \otimes |0\rangle \\ |01\rangle &\equiv |0\rangle \otimes |1\rangle \\ |10\rangle &\equiv |1\rangle \otimes |0\rangle \\ |11\rangle &\equiv |1\rangle \otimes |1\rangle \end{aligned}, \quad \text{where } \{|0\rangle, |1\rangle\}$$

is orthonormal
 basis for $\mathcal{H}_2^{(1)}$ and $\mathcal{H}_2^{(2)}$

carries \hat{A} and \hat{B} respectively
 (have left out superscripts (1) and (2))

- Thus for $|\psi\rangle \in \mathcal{H}_4$
 and $\hat{C} = \hat{A} \otimes \hat{B} \in \mathcal{L}(\mathcal{H}_4)$

$$|\psi\rangle = \sum_{k=0}^3 c_k |k\rangle, \quad \text{where } |k\rangle \equiv |k_1 k_2\rangle, \quad \text{where } k_1, k_2 \text{ is binary representation of } k$$

$$= c_0 |00\rangle + c_1 |01\rangle + c_2 |10\rangle + c_3 |11\rangle$$

$$= c_0 |0\rangle + c_1 |1\rangle + c_2 |2\rangle + c_3 |3\rangle$$

Tensor product (or Kronecker product) as the two vector spaces (with minimal constraints)

and

$$\begin{aligned} \hat{C}|\psi\rangle &= \hat{C} \sum_{k=0}^3 c_k |k\rangle = \sum_{k=0}^3 c_k \hat{C}|k\rangle \\ &= \sum_{k=0}^3 c_k \hat{A} \otimes \hat{B} |k\rangle \\ &= \sum_{k=0}^3 c_k \hat{A} |k_1\rangle \otimes \hat{B} |k_2\rangle \end{aligned}$$

Examples of two-qubit gates

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

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

ex. • construct the above matrix representations
 • CNOT for qubit 1 as target

n-qubit system

Formal definition
 $N \equiv 2^n = \dim\{\mathcal{H}_{2^n}\}$

$$\mathcal{H}_{2^n} = \mathcal{H}_2^{(1)} \otimes \mathcal{H}_2^{(2)} \otimes \dots \otimes \mathcal{H}_2^{(n)}$$

$$|\psi\rangle = \sum_{k=0}^{2^n-1} c_k |k\rangle = c_0 |0 \dots 0\rangle + c_1 |0 \dots 0 1\rangle + \dots$$

$\hat{I} \otimes \dots \otimes \hat{A} \otimes \hat{I} \otimes \dots \otimes \hat{I}$ is a single-qubit operator for qubit n

Quantum algorithms for n qubits

1. Initialize qubits to $|0\rangle$ (not necessarily all qubits)
2. Apply a desired n-qubit gate U (can be constructed from single and two-qubit gates)
3. Measure qubits (not necessarily all qubits)
4. Use measurement data and go to 1, unless algorithm finished

* In the simplest case one goes only once through 1-4, and initializes and measures all qubits in 1. and 3., respectively.

ex.

Deutsch algorithm

Entanglement for two qubits

- A quantum state of two qubits is defined entangled iff it cannot be represented as a product of two single-qubit states
- Thus $|\psi\rangle \in \mathcal{H}_1$ that are not entangled $\exists |\psi_1\rangle \in \mathcal{H}_2^{(1)}$ and $|\psi_2\rangle \in \mathcal{H}_2^{(2)}$

$$\text{s.t. } |\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle$$

- Examples of so-called maximally entangled states.

$$\text{Bell states } |\Phi^{\pm}\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$$

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

Commuting operators

- Let $\hat{A}, \hat{B} \in \mathcal{L}(\mathcal{H})$, $\hat{A} = \hat{A}^{\dagger}, \hat{B} = \hat{B}^{\dagger}$, and $[\hat{A}, \hat{B}] = 0$

thus it can be shown that

\exists complete eigenbasis of \hat{A} , that is also an eigenbasis of \hat{B} .

- Especially is $[\hat{A}, \hat{U}(t)] = 0 \quad \forall t$ the eigenvalues of \hat{A} are referred to as conserved quantities since we have $\hat{A}|\psi(t)\rangle = \hat{A}\hat{U}(t)|\psi(0)\rangle = \hat{U}(t)\hat{A}|\psi(0)\rangle = \lambda\hat{U}(t)|\psi(0)\rangle = \lambda|\psi(t)\rangle$

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

Prove according to exercise 3.1.(b)

Easy for formally constant Hamiltonians $\hat{A}e^{-i\hat{H}t} = e^{-i\hat{H}t}\hat{A}e^{i\hat{H}t} = e^{-i\hat{H}t}\hat{A}e^{i\hat{H}t} = \hat{A}$

Lecture 6 (last from Mihko)

ILOs

1. Identify Heisenberg's uncertainty relation.
2. Apply creation and annihilation operators for a harmonic oscillator.
3. Apply canonical commutation relations

Uncertainty relations

- Heisenberg's uncertainty relation states that $\Delta q \Delta p \geq \frac{\hbar}{2}$, where $\Delta A = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$, $[\hat{q}, \hat{p}] = i\hbar$ since \hat{q} and \hat{p} are "canonical conjugate pair"

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

- Robertson uncertainty relation

$$\Delta A \Delta B \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|, \text{ when } \hat{A}, \hat{B} \in \mathcal{L}(\mathcal{H})$$

unbounded, $\hat{A} = \hat{A}^\dagger, \hat{B} = \hat{B}^\dagger$

and $\langle \cdot \rangle = \langle \psi | \cdot | \psi \rangle$

• Let us define $|s\rangle = (\hat{A} - \langle \hat{A} \rangle) |\psi\rangle$
and $|g\rangle = (\hat{B} - \langle \hat{B} \rangle) |\psi\rangle$

$$\begin{aligned} \Delta A^2 &= \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle \\ &= \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^\dagger (\hat{A} - \langle \hat{A} \rangle) | \psi \rangle \\ &= \langle (\hat{A} - \langle \hat{A} \rangle) \psi | (\hat{A} - \langle \hat{A} \rangle) \psi \rangle \end{aligned}$$

$$= \langle s | s \rangle = \| |s\rangle \|^2$$

$$\Delta B^2 = \langle g | g \rangle = \| |g\rangle \|^2$$

Thus Cauchy inequality implies

$$|\langle s | g \rangle| \leq \| |s\rangle \| \| |g\rangle \|$$

$$\Rightarrow \Delta A \Delta B \geq |\langle s | g \rangle|$$

$$= |\langle \psi | (\hat{A} - \langle \hat{A} \rangle)^\dagger (\hat{B} - \langle \hat{B} \rangle) | \psi \rangle|$$

$$\geq |\langle \psi | (\hat{A} - \langle \hat{A} \rangle)^\dagger (\hat{B} - \langle \hat{B} \rangle) | \psi \rangle| = \frac{|\langle \psi | (\hat{B} - \langle \hat{B} \rangle)^\dagger (\hat{A} - \langle \hat{A} \rangle) | \psi \rangle|^2}{4}$$

$$= |\langle \psi | [\hat{A} - \langle \hat{A} \rangle, \hat{B} - \langle \hat{B} \rangle] | \psi \rangle|^2 / 4$$

$$= |\langle [\hat{A}, \hat{B}] \rangle|^2 / 4 \quad \square$$

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

One-dimensional quantum harmonic oscillator

As we derived earlier

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

$\omega = \frac{m\omega}{m} = \omega$

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

try writing using $A, B, C \in \mathbb{R}$

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

$$= A^2 \hat{q}^2 + iAB \hat{q}\hat{p} - iB\hat{p}A\hat{q} + B^2 \hat{p}^2 + C$$

$$= A^2 \hat{q}^2 + B^2 \hat{p}^2 + iAB \underbrace{[\hat{q}, \hat{p}]}_{i\hbar} + C$$

$$= \hbar BA$$

choose

$$A = \sqrt{\frac{1}{2} m \omega^2}$$

$$B = \sqrt{\frac{1}{2m}}$$

$$C = \hbar \omega$$

$$= \frac{\hbar \omega}{2}$$

$$= \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{q}^2$$

$$= \left(\hat{q} \sqrt{\frac{m\omega^2}{2}} + i\hat{p} \sqrt{\frac{1}{2m}} \right) \left(\hat{q} \sqrt{\frac{m\omega^2}{2}} - i\hat{p} \sqrt{\frac{1}{2m}} \right) + \frac{1}{2} \hbar \omega$$

$$= \hbar \omega \left[\underbrace{\sqrt{\frac{m\omega^2}{2}} \hat{q} + \frac{i}{m\omega} \hat{p}}_{\hat{a}^\dagger} \underbrace{\sqrt{\frac{m\omega^2}{2}} \hat{q} - \frac{i}{m\omega} \hat{p}}_{\hat{a}} + \frac{1}{2} \right]$$

math

$$(x-y)(x+y) = x^2 - y^2, \quad x, y \in \mathbb{R}$$

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

$$z^* = -iy$$

$$\sqrt{\frac{\hbar \omega}{2m}} \sqrt{\frac{m\omega}{2\hbar}} = \sqrt{\frac{\hbar m \omega^2}{2\hbar}} = \sqrt{\frac{m\omega^2}{2}}$$

$$\sqrt{\frac{\hbar \omega}{2m}} \frac{1}{m\omega} = \sqrt{\frac{m\omega^2}{2}} \frac{1}{m\omega} = \sqrt{\frac{m\omega^2}{2m^2\omega^2}} = \sqrt{\frac{1}{2m}}$$

$$\Rightarrow \hat{H} = \hbar \omega \left(\hat{a}^\dagger + \hat{a} + \frac{1}{2} \right), \text{ where}$$

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

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

Let us calculate

$$[\hat{a}, \hat{a}^\dagger] = \frac{m\omega}{2\hbar} \left[\hat{q} + \frac{i}{m\omega} \hat{p}, \hat{q} - \frac{i}{m\omega} \hat{p} \right]$$

$$= \frac{m\omega}{2\hbar} \left([\hat{q}, -\frac{i}{m\omega} \hat{p}] + [\frac{i}{m\omega} \hat{p}, \hat{q}] \right)$$

$$= \frac{i}{2\hbar} \left(-\underbrace{[\hat{q}, \hat{p}]}_{i\hbar} + \underbrace{[\hat{p}, \hat{q}]}_{-i\hbar} \right) = 1$$

• Observations:

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

since $\langle \psi | \frac{1}{2} \omega (\hat{a}^\dagger \hat{a} + \frac{1}{2}) | \psi \rangle = \langle \hat{H} \rangle$

$$= \frac{1}{2} \omega + \langle \psi | \frac{1}{2} \omega \hat{a}^\dagger \hat{a} | \psi \rangle$$

$$= \frac{1}{2} \omega (1 + \|\hat{a}|\psi\rangle\|^2) \geq 0$$

Thus all eigenenergies are positive.

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

$$\hat{H}|\psi\rangle = \epsilon|\psi\rangle, \quad \forall \psi$$

$$\hat{H} \hat{a} |\psi\rangle = \frac{1}{2} \omega (\hat{a}^\dagger \hat{a} + \frac{1}{2}) \hat{a} |\psi\rangle$$

$$= \hat{a} \hat{a}^\dagger - 1$$

$$= \hat{a} \left[\frac{1}{2} \omega (\hat{a}^\dagger \hat{a} + \frac{1}{2} - 1) |\psi\rangle \right]$$

$$= \hat{a} (\epsilon - \frac{1}{2} \omega) |\psi\rangle = (\epsilon - \frac{1}{2} \omega) \hat{a} |\psi\rangle$$

1. $\psi \neq 0 \Rightarrow \exists |0\rangle \in \mathcal{H}$
 s.t. $\hat{a}|0\rangle = 0$

• $|0\rangle$ is the ground state, i.e., the state with the lowest energy

$$\hat{H}|0\rangle = \frac{1}{2} \omega (\hat{a}^\dagger \hat{a} + \frac{1}{2}) |0\rangle$$

$$= \frac{1}{2} \omega |0\rangle$$

$$\Rightarrow \epsilon_0 = 0$$

$$\hat{H} \hat{a}^\dagger |\psi\rangle = (\epsilon + \frac{1}{2} \omega) |\psi\rangle,$$

when $\hat{H}|\psi\rangle = \epsilon \cdot \psi$.

Thus spectrum of \hat{H} is

$$\{\epsilon_n\} = \left\{ \frac{1}{2} \omega (n + \frac{1}{2}) \right\}$$

with eigenstates $\{|n\rangle\}$.

that is $\hat{H}|n\rangle = \frac{1}{2} \omega (n + \frac{1}{2}) |n\rangle$

Symbolic operator differential

- let \hat{q} and \hat{p} be a conjugate pair and \hat{q} has a continuous spectrum.

Thus we have

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

and this satisfied by symbolically defining $\hat{p} = -i\hbar \partial_{\hat{q}}$, where

$\partial_{\hat{q}}$ means that we take

symbolically a derivative w.r.t. \hat{q} .

example

$$\forall |\psi\rangle \in \mathcal{H}$$

$$\partial_{\hat{q}} f(\hat{q}) |\psi\rangle$$

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

where f is a continuously differentiable function and f' means its derivative

Let us check the claim

$$[\hat{q}, \hat{p}] = \hat{q}\hat{p} - \hat{p}\hat{q}$$

$$= \hat{q}(-i\hbar \partial_{\hat{q}}) - (-i\hbar \partial_{\hat{q}})\hat{q}$$

$$= -i\hbar \hat{q} \partial_{\hat{q}} + i\hbar \partial_{\hat{q}} \hat{q}$$

$$= -i\hbar \hat{q} \partial_{\hat{q}} + i\hbar (\underbrace{\partial_{\hat{q}} \hat{q}}_{=I}) + i\hbar \hat{q} \partial_{\hat{q}}$$

$$= i\hbar \quad \checkmark$$

added after lecture

Solving the ground state in position representation

We know that $\hat{a}|0\rangle = 0$

$$0 = \langle x' | \hat{a} | 0 \rangle = \int dx \langle x' | \hat{x} + \frac{i}{m\omega} \partial_x \rangle | 0 \rangle$$

$$= \sqrt{\frac{m\omega}{2\hbar}} \int dx \langle x' | \hat{x} \rangle \left(\tilde{x} + \frac{\hbar}{m\omega} \partial_{\tilde{x}} \right) \psi_0(\tilde{x})$$

$$= \delta(\tilde{x} - x')$$

$$= \langle x' | 0 \rangle$$

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

$$\Rightarrow \psi_0(x) = C e^{-\frac{x^2 m \omega^2}{2\hbar}}$$

$\psi_0 \propto |0\rangle \dots$ \uparrow normalization coefficient = $(\frac{m\omega}{\pi\hbar})^{1/4}$