LECTURE 1

INTRODUCTION

08/09/2023

OUTLINE:
- Schrödinger's eq; atoms & molecules
- Density Functional Theory
- Quantum info, channel., processing.

REVIEW:

	CLASSICAL MECHANICS	QUANTUM MECHANICS
STATE SPACE	$\mathbb{R}^{3n}_x \times \mathbb{R}^{3n}_p$	$L^2(\mathbb{R}^{3n}_x)$
EVOLUTION	Hamiltonian / Newton's eq.	Schrödinger's equation
OBSERVABLES	Real fcts. on $\mathbb{R}^{3n}_x \times \mathbb{R}^{3n}_p$	Self-adjoint operators on $L^2(\mathbb{R}^{3n}_x)$
INTERPRETATION OF MEASUREM.	Deterministic	Probabilistic

* **STATE SPACE**: State of particle is given by square-integrable functions in the space:

$$L^2(\mathbb{R}^3) = \left\{ \psi : \mathbb{R}^3 \to \mathbb{C} : \int_{\mathbb{R}^3} |\psi(x)|^2 \, dx < \infty \right\}$$

Lebesgue space (also Hilbert space)

In this course, usually smooth & continuous fcts, so Riemann & Lebesgue integrals agree.

FACTS:

(1) $L^2(\mathbb{R}^3)$ is a vector space (i.e., $\psi, \phi \in L^2 \Rightarrow \alpha\psi + \beta\phi \in L^2 \ \forall \alpha, \beta \in \mathbb{C}$).

Pf:

$$\int |\psi + \phi|^2 \leq 2 \int (|\psi|^2 + |\phi|^2) = 2\int |\psi|^2 + 2\int |\phi|^2 < \infty .$$

(2) L^2 is a normed space with the standard L^2-norm: for $f \in L^2$,

$$\|f\|_2 = \left(\int |f|^2 \right)^{1/2} .$$

$\left(\|f\|_2 = 0 \Leftrightarrow f = 0 \text{ a.e.}; \ \|f+g\|_2 \leq \|f\|_2 + \|g\|_2 ; \ \|f\|_2 \geq 0 \ \forall f \right)$

(3) L^2 is Banach; i.e., it is a complete normed space.

That is, every Cauchy seq. is convergent; i.e.,

$$\|f_n - f_m\|_2 \to 0 \Rightarrow \exists f \in L^2 \text{ s.t. } \lim f_n = f.$$

(4) L^2 is a Hilbert space ! That is, L^2 norm induces an inner product:

$$\langle f, g \rangle = \int \bar{f} g$$

s.t.

- $\langle f, f \rangle \geq 0 \ \forall f \in L^2$ and $= 0 \Leftrightarrow f = 0$.
- linear in g, real linear in f.
- $\langle f, g \rangle = \overline{\langle g, f \rangle}$.

E.g., $f \perp g \Rightarrow \langle f, g \rangle = 0$

$f \parallel g \Rightarrow \langle f, g \rangle = \pm \|f\| \|g\|$

$\|f\| = \sqrt{\langle f, f \rangle}$

(5) Cauchy - Schwarz : $\boxed{|\langle f, g\rangle| \leq \|f\| \, \|g\|}$.

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* **DYNAMICS**: Governed by Schrödinger's eq.:

$$\text{(SE)} \qquad \boxed{i\hbar\,\partial_t \psi = -\frac{\hbar^2}{2m}\Delta_x \psi + V\psi}\,,$$

where $\hbar = h/2\pi \approx 6.6 \cdot 10^{-27}$ erg sec ; m = mass of particle ;

$$\Delta_x = \sum_{j=1}^{3} \partial_{x_j}^2 \ ;$$

$(V\psi)(x,t) = V(x)\,\psi(x,t)$ where $V(x)$ is the potential. Convenient notation:

$$V : L^2 \ni \psi(x) \longmapsto V(x)\,\psi(x,t) \in L^2$$

$$\Delta : \psi(x,t) \longmapsto \sum_j \partial_{x_j}^2 \psi(x,t)$$

$$\psi : \mathbb{R}^3_x \oplus \mathbb{R}_t \longrightarrow \mathbb{C} \quad \text{s.t.} \quad \|\psi(x,t)\|_2 < \infty \ \forall t$$

Wavefct. ψ is a path in $L^2(\mathbb{R})$

PROPERTIES OF ψ: $\psi \in L^2$ s.t. $\Delta\psi \in L^2$ and $\partial_t \psi \in L^2$
(i.e., $\psi \in H^2(\mathbb{R}^3)$).

Sobolev space of order 2.

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* **PROPERTIES OF (SE):**

(1) CAUSALITY: If $\psi(\cdot, t_0)$ is known, then (by uniqueness) we can find $\psi(\cdot, t_1)$, $t_1 > t_0$.

(2) SUPERPOSITION PRINCIPLE: If ψ and ϕ are solutions to (SE), then $\alpha\psi + \beta\phi$ is also a solution to (SE) $\forall \alpha, \beta \in \mathbb{C}$.

this means (SE) is a linear PDE

INTERPRETATIONS OF ψ: $i\hbar\,\partial_t \psi = \frac{\hbar^2}{2m}\Delta\psi + V\psi$.

Wavefct. ψ yield the probability of measuring some observable.

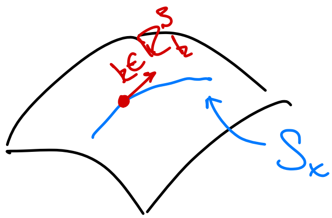
- For example, let $\Omega \subset \mathbb{R}^3$. Then,

$$\underbrace{\mathrm{Prob}_\psi(x \in \Omega)}_{\text{Prob. of measuring position of particle to be inside } \Omega \subset \mathbb{R}^3} = \int_\Omega |\psi|^2$$

[ASIDE: Normalize $\|\psi\|_2^2 = \int_{\mathbb{R}^3} |\psi|^2 \doteq 1$.]

- For example: probability of particle having momentum $\Omega \subset \mathbb{R}^3_k$ is given by

$$\mathrm{Prob}_\psi(\text{momen.} \in \Omega) = \int_\Omega |\underbrace{\hat{\psi}}_{\text{Fourier transform of } \psi}|^2$$



- $|\psi(x,t)|^2$ = Probability distribution for x at t.

* NOTE: • (SE) is linear, 2nd order, evolution PDE.

- (SE) can also be written as:

$$i\hbar\, \partial_t \psi = H\psi,$$

where

$$H : \psi(x,t) \longmapsto -\frac{\hbar^2}{2m} \Delta_x \psi(x,t) + V(x)\psi(x,t).$$

SCHRÖDINGER OPERATOR: $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$

linear

DIGRESSION INTO OPERATORS: Operators on $L^2(\mathbb{R}^3)$

- **Multiplication operator:**

$$M_V \,(\equiv V): \quad f(x) \longmapsto V(x) f(x)$$

- **Differentiation operator:**

$$\partial_{x_j}: \quad \psi(x) \longmapsto \partial_{x_j} \psi(x)$$

- **Laplacian operator:**

$$\Delta: \quad \psi \longmapsto \sum_j \partial_{x_j}^2 \psi \,.$$

- **Schrödinger operator:**

$$H = -\frac{\hbar^2}{2m} \Delta + V$$

As always... operator = rule & domain. An operator A on Hilbert space $\mathcal{H}$ $\to$ domain of A:

$$\boxed{D(A) := \{ f \in \mathcal{H} : Af \in \mathcal{H} \}}$$

!

domain of A

- $D(M_V) = L^2(\mathbb{R}^3)$ if V is $\underbrace{\text{bounded}}$.

  $f \in L^2 \Rightarrow Vf \in L^2$

- $D(\partial_{x_j}) = \{ f \in L^2 : \partial_{x_j} f \in L^2 \}$.

Note: $f \sim |x|^{-1} e^{-|x|} \in L^2(\mathbb{R}^3)$, $\partial_{x_j} f \notin L^2$.

Sobolev space of order 2

- $D(\Delta) = \{ f \in L^2 : \Delta f \in L^2 \} =: H^2(\mathbb{R}^3)$

e.g., $D(\Delta^2) = \{ f \in L^2 : \Delta^2 f \in L^2 \} =: H^4(\mathbb{R}^3)$.

- $D(M_{|x|^2}) = \{ f \in L^2 : \underbrace{|x|^2 f \in L^2} \}$.

operator of mult. by $|x|^2$

$\int |x|^4 |f|^2 < \infty$.

- Consider the operator $M_{|k|^2}$ in Fourier transform $(= |p|^2)$, where

$$|p|^2 : \psi(x) \longmapsto \overbrace{|k|^2 \hat{\psi}(k)}.$$

$\check{f}$ inverse FT of f:
$\check{f} = (2\pi)^{3/2} \int e^{-ik\cdot x} \psi(k) dx$

Then,

$$D(|p|^2) = \{ \psi \in L^2(\mathbb{R}^3_x) : |k|^2 \hat{\psi}(k) \in L^2(\mathbb{R}^3_k) \} = H^2(\mathbb{R}^3)$$

LECTURE 2

13/09/2023

CONSERVATION OF PROBABILITY

RECALL: Quantum dynamics is governed by (SE):

$$(SE) \quad i\hbar\, \partial_t \psi = H\psi, \quad \psi\big|_{t=0} = \psi_0$$

"CAUCHY PROBLEM"

where $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$ is the Schrödinger operator.

We say that ψ is the probability amplitude for each coördinate. Moreover,

$$|\psi(x,t)|^2 = \text{Probability distribution}$$

for x at a given time t.

Probability of particle w/ state ψ be found in $\Omega \subset \mathbb{R}^3$ is:

$$\text{Prob}(x \in \Omega) = \int_\Omega |\psi(x,t)|^2 \, dx.$$

Now, # of particles is fixed, so we expect that the total probability $\int_{\mathbb{R}^3} |\psi|^2 dx$ is independent of time t.

Claim: (CONSERVATION OF PROBABILITY) $\forall t \in \mathbb{R}$,

$$\int_{\mathbb{R}^3} |\psi(x,t)|^2 \, dx = \int_{\mathbb{R}^3} |\psi(x,0)|^2 \, dx$$

$\hookrightarrow$ Independent of particular quantum system.

Now: Consider (SE) on an arbitrary Hilbert space X with an abstract Schrödinger operator H acting on $\psi : \mathbb{R} \to X$.

Def: (SYMMETRIC OPERATOR) An operator H on a Hilbert space X is said to be symmetric iff $\forall \psi, \varphi \in D(H)$, $\leftarrow$ Domain of H

$$\langle \psi, H\varphi \rangle_X = \langle H\psi, \varphi \rangle_X .$$

Thm: If H is symmetric, then (SE) conserves "probability" in the sense that

$$\| \psi(t) \|_X = \| \psi(0) \|_X$$

$\|\cdot\|_X$ induced by $\langle \cdot, \cdot \rangle_X$

$\|\cdot\|_X = \sqrt{\langle \cdot, \cdot \rangle_X}$

EXAMPLES:

1) Multiplication by x_j is symmetric.

2) Multiplication by ix_j is not symmetric

← Changes sign on the $\langle \cdot, \cdot \rangle_X$

3) $P_j = -i\partial_{x_j}$ is symmetric.

However, ∂_{x_j} is not symmetric (by integration by parts)

4) Δ is symmetric

5) $K[\psi](x) := \int k(x,y)\,\psi(y)\,dy$ is symmetric provided that $k(x,y) = \overline{k(y,x)}$.

Pf: (Conservation of Probability)

($\Rightarrow$) Let H be symmetric. Then

$$\partial_t \|\psi(t)\|_X^2 = \partial_t \langle \psi(t), \psi(t) \rangle_X$$

Leibniz Rule

$$= \langle \dot{\psi}, \psi \rangle + \langle \psi, \dot{\psi} \rangle$$

(SE)

$$= \left\langle \frac{1}{i\hbar} H\psi, \psi \right\rangle + \left\langle \psi, \frac{1}{i\hbar} H\psi \right\rangle$$

Convention:
$\langle \alpha\psi, \phi \rangle = \bar{\alpha} \langle \psi, \phi \rangle$
$\langle \psi, \alpha\phi \rangle = \alpha \langle \psi, \phi \rangle$

$$= -\frac{1}{i\hbar} \langle H\psi, \psi \rangle + \frac{1}{i\hbar} \langle \psi, H\psi \rangle$$

H symmetric

$$= 0.$$

($\Leftarrow$) Conversely, if $\partial_t \|\psi(t)\|_X^2$, then

$$\langle H\psi(t), \psi(t) \rangle = \langle \psi(t), H\psi(t) \rangle$$

$$0 = \partial_t \|\psi(t)\|_X^2 = \langle \dot{\psi}, \psi \rangle + \langle \psi, \dot{\psi} \rangle =$$ same as the other direction

$\square$

* **DETOUR INTO OPERATORS:** Operator on a normed space X,

Def: (**BOUNDED OPERATOR**) An operator A is bounded on the space X iff $D(A) = X$ and $\forall u \in X$,

C is independent from $u \in X$.

$$\|Au\|_X \leq C \|u\|_X .$$

Then the smallest of such C's $:= \|A\|$

$$\iff \|A\| = \inf_{\forall u, \|u\|_X = 1} \|Au\|_X$$

$$\iff \boxed{\|A\| = \sup_{X \ni u \neq 0} \frac{\|Au\|_X}{\|u\|_X}}$$

PROPERTIES:

- $\|Au\|_X \leq \|A\| \|u\|_X$
- $\|AB\| \leq \|A\| \|B\|$

Ex: (i) Multiplication M_f by $f \in L^2(\mathbb{R}^m)$.
Then M_f is bdd $\iff$ f bdd a.e.

(ii) $\| M_f \|_{L^2} = \| f \|_{L^\infty} = \operatorname{ess\,sup} f \leq \sup_x |f(x)|$.

LECTURE 3

DYNAMICS

15/09/2023

Quantum evolution is defined by (SE):

$$i\hbar \, \partial_t \psi = H \psi , \quad \psi|_{t=0} = \psi_0$$

CAUCHY PROBLEM

$$H = -\frac{\hbar^2}{2m} \Delta_x + V$$

Assume $\psi_0 \in D(H)$

V always real for us
(b/c we need H to be symmetric)

First, consider the Cauchy Problem (SE)-(IC) in an abstract Hilbert space X and H an abstract operator.

Let $\psi : t \longmapsto \psi(t) \in D(H)$. In this setup, the time derivative of ψ is defined as

$$\partial_t \psi = \lim_{\varepsilon \to 0} \frac{\psi(t+\varepsilon) - \psi(t)}{\varepsilon}$$

(provided that lim exists). In particular, the limit is:

$$\left\| \partial_t \psi - \frac{1}{\varepsilon}\left(\psi(t+\varepsilon) - \psi(t)\right)\right\|_X \xrightarrow{\varepsilon \to 0} 0$$

NOTE: X Hilbert space $=$ X vector space, inner product and complete.

Complete normed space

i.e., Banach space whose norm is induced by an inner product.

Def: The dynamics exist if and only if the Cauchy problem $(SE)-(IC)_x$ has a <u>unique</u> solution in X $\forall \psi \in D(H)$ <u>and</u> this solution $\psi(t)$ satisfies conservation of probability in the X-norm; i.e., $\|\psi(t)\|_X = \|\psi(0)\|_X \quad \forall t$.

Claim: (last lecture) If H is symmetric, then <u>any</u> solution of $(SE)-(IC)$ satisfies conservation of probability $\|\psi(t)\|_X = \|\psi(0)\|_X$ $\forall t$.

Lemma: If H is symmetric, $\psi_0 \in D(H)$ and $\psi(t)$ is a solution to $(SE)-(IC)$, then

$$\psi(t) \in D(H) \quad \forall t.$$

Pf: <u>Claim</u>: $\partial_t \|H\psi(t)\|_X^2 = 0$.

This implies that $\|H\psi(t)\|_X = \|H\psi_0\|_X < \infty$

$\Rightarrow \psi(t) \in D(H) \quad \forall t.$

"Pf" of claim:

$$\partial_t \| H\psi(t) \|_X^2 = \partial_t \langle H\psi(t), H\psi(t) \rangle_X$$

$$\overset{\text{Leibniz}}{=} \langle H\dot{\psi}, H\psi \rangle_X + \langle H\psi, H\dot{\psi} \rangle_X$$

$$= \langle H\dot{\psi}, H\psi \rangle_X + \overline{\langle H\dot{\psi}, H\psi \rangle_X}$$

$$\overset{(SE)}{=} 2\,\mathrm{Re} \langle H\psi, H \tfrac{1}{i\hbar} H\psi \rangle_X$$

$$= \frac{2}{\hbar} \mathrm{Re}\, \frac{1}{i} \langle \underbrace{H\psi}_{=:\phi}, H \underbrace{H\psi}_{=:\phi} \rangle_X$$

$$= \frac{2}{\hbar} \mathrm{Re}\, \frac{1}{i} \langle \phi, H\phi \rangle_X$$

H symmetric $\Rightarrow \langle \phi, H\phi \rangle_X \in \mathbb{R}$ so, w/ the i multiplied, the real part is zero.

$$= 0$$

□

Obs: $$\partial_t H\psi(t) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} [H\psi(t+\varepsilon) - H\psi(t)]$$

$$\overset{\text{linearity}}{=} H \left(\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} [\psi(t+\varepsilon) - \psi(t)] \right)$$

$$= H (\partial_t \psi(t)).$$

Ex: $H = -\frac{\hbar^2}{2m}\Delta + V$, V real, is symmetric since Δ is symmetric and V is real (hence symmetric).

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* EXISTENCE OF SOLUTIONS TO (SE)-(IC)

Thm: The dynamics exist if and only if H is self-adjoint ($H = H^*$).

Claim: Properties of self-adjoint operators:

- $\boxed{H \text{ self-adjoint}} \Rightarrow \boxed{H \text{ symmetric}}$

  Converse not true in general

- $\boxed{H \text{ bounded and symmetric}} \Rightarrow \boxed{H \text{ self-adjoint}}$
- In QM, all symmetric operators are self-adjoint

Def: (ADJOINT) The adjoint of an operator A is denoted A^* and it satisfies

$$\boxed{\langle A^*\psi, \phi\rangle_X = \langle \psi, A\phi\rangle_X}$$

$\forall \psi \in D(A^*)$, $\phi \in D(A)$. Now,

$$D(A^*) = \{ \psi \in X : |\langle \psi, A\phi\rangle_X| \leq C_\psi \|\phi\|_X \}.$$

Prop:

(i) If A is bounded, then $D(A^*) = X$.

$\Downarrow$

(ii) If A is bounded and symmetric, then A is self adjoint.

Pf: (i) $\forall \phi \in X$, by Cauchy-Schwarz,

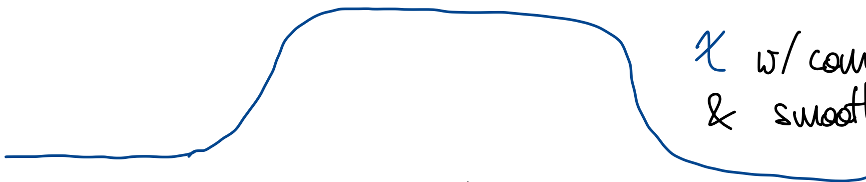
$$|\langle \psi, A\phi\rangle| \leq \|\psi\| \|A\phi\| \leq \underbrace{\|\psi\| \|A\|}_{=: C_\psi} \|\phi\|$$

A bounded $\Rightarrow \|A\phi\| \leq \|A\| \|\phi\|$

$\square$

Ex: **Claim**: $\exists \{\psi_n\} \subset L^2(\mathbb{R})$ s.t. $\|\psi_n\|_{L^2} = 1$ and $\|\Delta \psi_n\|_{L^2} \longrightarrow +\infty$ (i.e., Δ is unbounded)!

Take a sequence of ψ_n s.t.



χ w/ compact supp & smooth

Take $\psi_h(x) := \chi(x) e^{ik\cdot x/h}$. Then

$$\Delta \psi_h = \underbrace{(\Delta \chi) e^{ik\cdot x/h}}_{=f_1} + \underbrace{2\nabla\chi \cdot \underbrace{\nabla e^{ik\cdot x/h}}_{= \frac{ik}{h} e^{ik\cdot x/h}}}_{=f_2} + \underbrace{\chi \underbrace{\Delta e^{ik\cdot x/h}}_{= -\frac{|k|^2}{h^2} e^{ik\cdot x/h}}}_{=f_3}$$

Then, compute

$$\|\Delta \psi_h\|_{L^2} = \|f_1 + f_2 + f_3\|_{L^2}$$

Triangle ineq.

$$\geq \underbrace{\|f_3\|_{L^2}}_{|k|^2 \to +\infty} - \underbrace{\|f_1\|_{L^2}}_{O(1)} - \underbrace{\|f_2\|_{L^2}}_{O(|k|)}$$

Therefore, Δ is unbounded!

$\square$

* **KEY POTENTIALS IN QM:**

(1) $$\boxed{V(x) = \sum_j \frac{\alpha_j(x)}{|x - x_j|^{\beta_j}} + W(x),}$$

where α_j, W bounded and $\beta < 2$.

the above $V \implies H = H^*$

(2) $V \geq 0$, $V(x) \to \infty$ as $|x| \to \infty$, gives $H^* = H$.

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* **PROPAGATORS:** Basically a flow for (SE).

We have

$$\begin{cases} i\hbar \partial_t \psi = H\psi & (SE) \\ \psi(t=0) := \psi_0 & (IC) \\ \psi : t \longmapsto \psi(t) \in X, \ \psi_0 \in D(H) \end{cases}$$

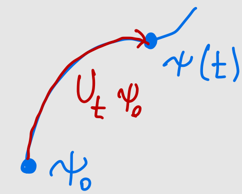
shown before

$\implies \forall \psi_0 \in D(H)$, $\exists!$ solution to (SE)-(IC) in $D(H)$ and $\|\psi(t)\|_X = \|\psi(0)\|_X \ \forall t$.

Def: (PROPAGATOR) A one-parameter family U_t of bounded operators is called a propagator for (SE) if it has the following properties:

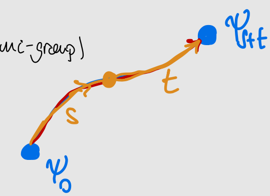
path in X

- Defined as $\boxed{U_t \psi_0 = \psi(t)}$.



- $\forall t$, U_t is bounded ($\boxed{\|U_t\|_X = 1}$).
- $\boxed{U_s U_t = U_{s+t}}$ and $\boxed{U_0 = \mathrm{Id}}$.

(semi-group)



In the strong sense

- $\boxed{i\hbar\, \partial_t U_t = H U_t}$. (Satisfies (SE))
- $\boxed{\langle U_t \phi, U_t \psi \rangle_X = \langle \phi, \psi \rangle_X}$. (Isometry)

$\Rightarrow U_t^{-1} = U_t^* \Rightarrow U_t$ is unitary

[**ASIDE**: Limits as $s \to 0$

- **UNIFORM**: $\|A_s - A_0\| \longrightarrow 0$

$\|$

- ! **STRONG**: $\|A_s\psi - A_0\psi\| \longrightarrow 0$

$\Downarrow$

- **WEAK**: $\langle \phi, A_s\psi \rangle \longrightarrow \langle \phi, A_0\psi \rangle$

$\forall \phi \in X,\ \forall \psi \in \bigcap_s D(A_s).$

So, there are 3 ways of taking limits, i.e., 3 notions of derivatives, i.e., 3 topologies]

Pf: • U_t bdd:

Conservation of probability

$$\|U_t\psi_0\|_X \overset{\text{def}}{=} \|\psi(t)\|_X = \|\psi_0\|_X$$

$$\Longrightarrow \|U_t\| = 1.$$

- Group property $U_sU_t = U_{s+t}$: follows from uniqueness (LHS and RHS satisfy the same equation w/ same (IC)).

- U_t satisfies (SE): from definition.

- $\underline{\langle U_t \phi, U_t \psi \rangle_X = \langle \phi, \psi \rangle_X}$: Same method of proof of conservation of probability. Note that $U_t \phi$ solves (SE) w/ initial condition $= \phi$ (b/c you evolved by t)

$\square$

$\boxed{\text{LECTURE 4}}$ QUANTUM OBSERVABLES

20/09/2023

Def: (PHYSICAL OBSERVABLE) A physical observable is a physical quantity measured in experiments.

e.g., position, momentum, angular momentum, energy, spin.

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__Recall__: A wavefct. $\psi(x,t)$ gives the __probability__ distribution $|\psi(x,t)|^2$ for position x of a particle.

Def: (AVERAGE POSITION) The average position at time t is given by

$$\int x\,|\psi(x,t)|^2\,dx = \int \bar{\psi}\,x\,\psi.$$

Def: (PROBABILITY)

$$\mathrm{Prob}_\psi(x \in \Omega) = \int_\Omega |\psi(x,t)|^2\,dx$$

$$= \int \bar{\psi}\,\chi_\Omega\,\psi\,dx$$

$\Rightarrow$ Can define the average position as:

$$\mathrm{Av}(x) \overset{\mathrm{def}}{=} \int x\,|\psi(x,t)|^2\,dx$$

$$= \langle \psi, M_x \psi \rangle,$$

!!

where M_x is multiplication by x defined as $M_x : \psi(x,t) \longmapsto x\,\psi(x,t)$.

Thus,

$$\mathrm{Prob}_\psi(x \in \Omega) = \langle \psi, M_{\chi_\Omega} \psi \rangle$$

$$= \langle \psi, \chi_\Omega(M_x)\psi \rangle ,$$

where

$$M_{\chi_\Omega(x)} : \chi_\Omega(M_x) \longmapsto M_{f(x)} = f(M_x)$$

Define $x := M_x$ <u>position operator</u>.

Suppose ψ_t is a solution to (SE). Then

$$\partial_t \langle \psi_t, x\psi_t \rangle$$

Lemma: Let A be an operator on a Hilbert space $\mathcal{H}$ and let ψ_t be a solution to (SE) w/ symmetric Schrödinger operator H $(i\hbar \partial_t \psi_t = H\psi_t)$.

Then

$$\partial_t \langle \psi_t, A\psi_t \rangle = \langle \psi_t, \frac{i}{\hbar}[H,A]\psi_t \rangle$$

Pf: (Lemma)

! IMPORTANT COMPUTATION !

! STUDY FOR TESTS

$$\partial_t \langle \psi_t, A\psi_t \rangle \overset{\text{Leibniz}}{=} \langle \dot{\psi}_t, A\psi_t \rangle + \langle \psi_t, A\dot{\psi}_t \rangle$$

$$\overset{(SE)}{=} \left\langle \frac{1}{i\hbar} H\psi_t, A\psi_t \right\rangle + \left\langle \psi_t, A\frac{1}{i\hbar} H\psi_t \right\rangle$$

$$= -\frac{1}{i\hbar} \langle \psi_t, [H,A]\psi_t \rangle .$$

$\square$

Ex: Compute commutator of

$$H = -\frac{\hbar^2}{2m}\Delta + V(x) \quad \text{and} \quad x_j$$

Then:

$$\frac{i}{\hbar}[H, x_j] = \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta, x_j\right]$$

$$\boxed{[M_f, M_g]\psi = (fg - gf)\psi = 0}$$

$$+ \cancel{\frac{i}{\hbar}[V, x_j]} = 0$$

$$= \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta, x_j\right]$$

$$\boxed{[\Delta, x_j]\psi = 2\partial_{x_j}\psi}$$

$$= \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\right) \cdot 2\partial_{x_j}$$

"Normalize the mass"

$$= -i\hbar\partial_{x_j} =: P_j$$

$(*)$

Def: (MOMENTUM OPERATOR) Momentum of the j-th coördinate is

$$P_j := -i\hbar\,\partial_{x_j}.$$

Upshot:

Lemma

$$\partial_t \langle \psi_t, x\psi_t\rangle = \left(\psi_t, \frac{i}{\hbar}[H, x_j]\psi_t\right)$$

$$\overset{(*)}{=} \left\langle \psi_t, \frac{1}{m} P_j \psi_t \right\rangle.$$

Therefore,

"Expectation value"

$$m\,\partial_t\, Av_{\psi_t}(x_j) = Av_{\psi_t} P_j,$$

where p is the momentum observable (or momentum operator), and x is the position observable (or operator).

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* **Differentiate Average Momentum**:

$$\partial_t \langle \psi_t, P_j \psi_t \rangle \overset{\text{Lemma}}{=} \left(\psi_t, \frac{i}{\hbar}[H, P_j]\psi_t \right)$$

$$\frac{i}{\hbar}[H, P_j] = \cancel{\frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\Delta, -i\hbar \partial_{x_j} \right]} \to = 0 \text{ (the derivatives commute)}$$

$$+ \frac{i}{\cancel{\hbar}}\left[V, -i\cancel{\hbar} \partial_{x_j} \right]$$

$$= -\partial_{x_j} V$$

$$[V, \partial_{x_j}]\psi = V\partial_{x_j}\psi - \partial_{x_j}(V\psi) - ((\partial_{x_j}V)\psi + V\partial_{x_j}\psi)$$

$$\Rightarrow \frac{i}{\hbar}[H, P] = -\nabla V$$

!!

Thus, EHRENFEST'S EQUATION

$$\partial_t \langle \psi_t, P_j \psi_t \rangle = \langle \psi_t, -\partial_{x_j} V \psi_t \rangle$$

——————— // ———————

Def: A physical observable is a self-adjoint (bounded) operator A on a Hilbert space $\mathcal{H}$ (e.g., $L^2(\mathbb{R}^3)$).

Def: (AVERAGE) The average of observable A on state ψ_t is defined as

$$\mathrm{Av}_{\psi_t}(A) := \langle \psi_t , A \psi_t \rangle .$$

Then, the evolution of the average is given by

$$\partial_t \mathrm{Av}_{\psi_t}(A) \underset{\text{by Lemma}}{=} \mathrm{Av}_{\psi_t}\left(\frac{i}{\hbar} [H, A] \right) .$$

NOTE: $$-\frac{\hbar^2}{2m} \Delta = \frac{1}{2m} |p|^2$$

(where $|p|^2 := \sum_j p_j^2 = -\hbar^2 \sum_j \partial_{x_j}^2 = -\hbar^2 \Delta$)

$\Rightarrow \quad H = \frac{1}{2m} |p|^2 + V$ which looks like a classical Hamiltonian.

Quantum Hamiltonian w/ observable energy

Lecture 5 — Quantum Observables

22/09/2023

Recall: From last lecture,

$\boxed{\text{Quantum observables}} = \boxed{\text{Operators representing physical operators}}$

Examples:

- **Position operator**: Multiplication by x (M_x)
- **Momentum operator**: $P_j := -i\hbar \partial_{x_j}$
- **Energy operator**: Schrödinger operator

$$H = -\frac{\hbar^2}{2m}\Delta + V(x)$$

! In general, observables are represented by self-adjoint operators on $L^2(\mathbb{R}^3)$.

— // —

or expectation values

* **TIME EVOLUTION OF AVERAGES**: Suppose ψ_t is a solution to (SE) and that

$$\langle A \rangle_\psi \overset{\text{def}}{=} \langle \psi, A\psi \rangle$$

is the average (or expectation value) of A in the state ψ. Then,

$$\partial_t \langle x \rangle_{\psi_t} = \frac{1}{m} \langle p \rangle_{\psi_t}$$

$$\partial_t \langle p \rangle_{\psi_t} = \langle -\nabla V \rangle_{\psi_t}$$

!! In general: $\partial_t \langle A \rangle_{\psi_t} = \left\langle \frac{i}{\hbar}[H, A] \right\rangle_{\psi_t}$.

* **CONSERVATION LAWS**: Note that $\langle \phi, A\psi \rangle$ is called the matrix element of A in ϕ and ψ.

Now,

(i.e., $\partial_t \langle \phi_t, A\psi_t \rangle = 0$)

$$\boxed{\text{Observable } A \text{ is conserved}} \iff \boxed{\langle \phi_t, A\psi_t \rangle \text{ is independent of time } \forall \phi_t, \psi_t \text{ solutions to (SE)}}$$

Lemma:

$$\boxed{\text{Observable } A \text{ is conserved}} \iff \boxed{[H, A] = 0}$$

Pf: Similar to $\partial_t \langle \phi_t, A\psi_t \rangle = \langle \phi_t, \frac{i}{\hbar}[H,A]\psi_t \rangle$

($\Rightarrow$) If A is conserved, then

$$\partial_t \langle \phi_t, A\psi_t \rangle = 0 \Rightarrow \langle \phi_t, [H,A]\psi_t \rangle = 0$$

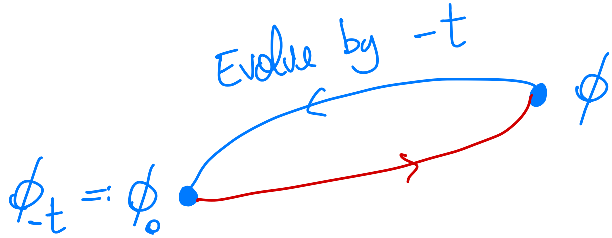
$\forall \phi_t, \psi_t \in L^2(\mathbb{R}^3)$

Properties of $\langle \cdot, \cdot \rangle_{L^2}$

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

Claim: $\forall \phi \in L^2(\mathbb{R}^3)$ $\exists t \in \mathbb{R}$, $\phi_0 \in L^2(\mathbb{R}^3)$ s.t. $\phi = \phi_t$ solves (SE) with initial condition ϕ_0.

Pf: Just take ϕ as the initial condition; use existence & uniqueness; move backwards in time by t and find ϕ_0. Then redefine time so that ϕ_0 is the initial condition. That is:



($\Leftarrow$) Tautology using Ehrenfest. ∎

—— // ——

* **EXAMPLES OF CONSERVED OBSERVABLES:**

(1) $A = H$. Obviously, $[H, H] = 0$

$\Rightarrow$ Conservation of energy!

(2) $A = \mathrm{Id}$. Obviously $[H, \mathrm{Id}] = 0$.

$\Rightarrow$ Conservation of total probability!

$0 = \partial_t \langle \phi_t, \mathrm{Id}\, \psi_t \rangle \Rightarrow \langle \phi_t, \psi_t \rangle$ is indep. of time

(3) $A = x_j$. Compute:

as before

$\frac{i}{\hbar}[H, x_j] = p_j \Rightarrow \langle \phi, p_j \psi \rangle \neq 0$ for some ϕ, ψ.

$\Rightarrow$ Position is <u>not</u> conserved!

(4) $A = p_j$. Then, as before,

$$\frac{i}{\hbar}[H, p_j] = -\partial_{x_j} V.$$

Thus, p_j is conserved $\Longleftrightarrow$ V is independent of x_j

$\Longleftrightarrow$ V is invariant under x_j – translations.

$V(x)$ needs some symmetries

(5) $A = L$, where $L := p \wedge x = -x \wedge p$

ANGULAR MOMENTUM OPERATOR

Then,

$$\frac{i}{\hbar}[H, L] = -(LV) = 0$$

$\Updownarrow$

isometries in $\mathbb{R}^3$

V is rotationally invariant
(i.e., $V(Rx) = V(x)\ \forall R \in O(3)$)
(i.e., $V(x) = \tilde{V}(|x|)$).

<u>HW</u>: Show that

$$A(t) \text{ conserved} \iff \frac{i}{\hbar}[H, A(t)] + \partial_t A(t) = 0$$

— // —

<u>Claim</u>: Conservation of probability

$\Updownarrow$

Gauge symmetry

$U_\alpha : \psi(x,t) \mapsto e^{i\alpha}\psi(x,t)$
$e^{i\alpha} \in U(1)$

FUN ASIDE: Consider a particle moving in a magnetic field $B(x)$ (constant in time). Let $A(x)$ be the vector potential for the magnetic field; i.e., $B = \text{curl } A$.

In this case, the classical Hamiltonian

Lower case = classical

$$h(x,k) = \frac{1}{2m}|k - eA(x)|^2 + V(x).$$

The quantum Hamiltonian is given by

$$H = \frac{1}{2m}|p - eA(x)|^2 + V(x).$$

Now, from gauge invariance

$$\psi \longmapsto e^{i\alpha}\psi$$

α is any differentiable fct.

$$A \longmapsto A + \nabla\alpha$$

$\forall x \in \mathbb{R}^3$, $\alpha(x) \in U(1)$

* **HEISENBERG'S EQUATIONS**: Let A be an observable and ϕ_t, ψ_t be solutions to (SE).

Lemma: (HEISENBERG REPRESENTATION)

$$\langle \phi_t, A\psi_t \rangle = \langle \phi_0, A(t)\psi_0 \rangle,$$

where $A(t)$ satisfies

$$\left.\partial_t A(t) = \frac{i}{\hbar}[H, A(t)]\right\} \text{HEISENBERG EQUATION}$$

Pf: (HOMEWORK) Idea is to consider the propagator $\psi_t = U_t\psi_0$. Then U_t applied to ψ_0 gives

$$\langle \phi_t, A\psi_t \rangle = \langle U_t\phi_0, AU_t\psi_0 \rangle$$

Assume U_t a bdd $\forall t$

$$= \langle \phi_0, U_t^* A U_t \psi_0 \rangle$$

Define $A(t) := U_t^* A U_t$

$$= \langle \phi_0, A(t)\psi_0 \rangle.$$

Left to show that $A(t)$ satisfies Heisenberg's eq.

Use $i\hbar\partial_t U_t = HU_t \Rightarrow -i\hbar\partial_t U_t^* = HU_t^*$. $\leftarrow (AB)^* = B^*A^*$ ■

- HEISENBERG EQUATIONS FOR x & p:

$$\begin{cases} \partial_t x(t) = \frac{i}{\hbar}[H, x(t)] \overset{(I)}{=} \frac{1}{m} p(t) \\ \partial_t p(t) \overset{(II)}{=} -(\nabla V)(t) \end{cases}$$

Claim: (Equivalent Heisenberg Equation)

$$\partial_t A(t) = \left(\frac{i}{\hbar}[H,A]\right)(t)$$

Pf:

$$\partial_t A(t) = \dot{U}_t^* A U_t + U_t^* A \dot{U}_t$$

$$= \frac{1}{i\hbar}\left(-U_t^* HA U_t + U_t^* AHU_t\right)$$

$$= \frac{i}{\hbar} U_t^* (HA - AH) U_t$$

$$= \frac{i}{\hbar} U_t^* [H,A] U_t .$$

$\blacksquare$

So, now compute $\partial_t x(t)$ and $\partial_t p(t)$:

(I): $\frac{i}{\hbar}[H, x] = p \rightsquigarrow \boxed{\partial_t x(t) = \frac{1}{m} p(t)}$

(II): $\frac{i}{\hbar}[H, p] = -\nabla V \rightsquigarrow \boxed{\partial_t p(t) = (-\nabla V)(t)}$

QUANTUM HAMILTON'S EQS.

Quite similar to the classical Hamilton eq.

A classical operator a evolves according to

$$\partial_t a = \{h, a\} \rightarrow \{f, g\} = \nabla_k f \nabla_x g - \nabla_x f \nabla_k g$$

Poisson bracket

$\{h, a\} \rightarrow \frac{i}{\hbar}[H, A]$ QM

$$\partial_t A = \frac{i}{\hbar}[H, A]$$

* PROBABILISTIC INTERPRETATION:

$$\boxed{\mathrm{Prob}_\psi(\text{norm} \in \Omega) = \int_\Omega |\hat{\psi}(k,t)|^2 \, dk}$$

Fourier transform

• FOURIER TRANSFORM:

Defined as

$$\hat{\psi}(k) := (\mathcal{F}\psi)(k)$$

$$:= (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^3} \psi(x)\, e^{-ik\cdot x/\hbar} \, dx$$

Inverse Fourier Transform

$$\check{\phi}(x) := (2\pi\hbar)^{-n/2} \int_{\mathbb{R}^3} \phi(k)\, e^{ik\cdot x/\hbar} \, dk$$

PROPERTIES:

(1) $\widehat{P_j \psi} = k_j \hat{\psi}(k)$; $\widehat{x_j \psi} = i\hbar \nabla_k \hat{\psi}$

(2) $\langle \hat{\phi}, \hat{\psi} \rangle = \langle \phi, \psi \rangle = \langle \check{\phi}, \check{\psi} \rangle$.

LECTURE 6

27/09/2023

QUANTIZATION

	CLASSICAL MECHANICS	QUANTUM MECHANICS
STATE SPACE	n particles $\mathbb{R}^n_x \times \underbrace{\mathbb{R}^n_k}_{T_p(\mathbb{R}^n_x)}$ $= TM$ tangent bundle	$L^2(\mathbb{R}^n_x)$ n particles
OBSER-VABLES	fcts. of the form $f(x,k)$	Self-adjoint operators on the state space
DYNA-MICS	$\{f,g\} = \nabla_k f \nabla_x g - \nabla_x f \nabla_k g$ $h(x,k) \rightsquigarrow$ Hamiltonian fct. $\Rightarrow \partial_t a = \{h, a\}$ "Liouville Equation"	Commutator $\frac{i}{\hbar}[B,A]$ $\Rightarrow \partial_t A = \frac{i}{\hbar}[H,A]$ "Heisenberg Equation"

Canonical variables:

Variables	Operators
x_j, k_j	$x_j, p_j \ (:= -i\hbar \partial_{x_j})$
$\{x_j, k_j\} = \delta_{ij}$	$\frac{i}{\hbar}[x_j, p_j] = \delta_{ij}$

Dynamics for canonical variables:

$$\partial_t x_j = \frac{k_j}{m} \qquad \partial_t x_j = \frac{P_j}{m}$$

potential

$$\partial_t k_j = -\partial_{x_j} V(x) \qquad \partial_t P_j = -\partial_{x_j} V(x)$$

HAMILTON'S EQUATIONS

EHRENFEST-HEISENBERG EQUATIONS

- **Properties of the Poisson bracket $\{\cdot,\cdot\}$:**

(i) $\{f, g\}$ is linear in f and g

(ii) $\{f, g\} = -\{g, f\}$ (antisymmetry)

(iii) $\{f, gh\} = \{f, g\}h + g\{f, h\}$

(iv) Jacobi's identity.

These are defining properties of $\{\cdot,\cdot\}$.

* QUANTIZATION

Canonical variables $\rightsquigarrow$ Operators

$$(x, \xi) \rightsquigarrow (x = M_x, \; p = -i\hbar\nabla)$$

Classical object a written in terms of canonical variables:

$$a(x,\xi) \rightsquigarrow \underbrace{A := a(M_x, p)}_{\text{Pseudo-differential operator on } L^2(\mathbb{R}^n)}$$

$\boxed{\text{Ex}}$: (Quantizations)

(1) Classical angular momentum $\ell := x \wedge \xi$

$$\rightsquigarrow$$

$$L = x \wedge P$$

(2) Classical Hamiltonian

$$h(x,\xi) = \frac{1}{2m}|\xi|^2 + V(x)$$

$$\rightsquigarrow$$

$$H(x,p) = \frac{1}{2m}|p|^2 + V(x) \text{ in } L^2(\mathbb{R}^3)$$

PROBLEM : $x_1 k_1 \to x_1 p_1$ or $p_1 x_2$

or $\frac{1}{2}(x_1 p_1 + p_1 x_1)$] "Weyl Quantization"

But don't worry about this now ☺

$\boxed{\text{Ex}}$: (Particle in EM-field) Described by vectors and scalars. Suppose we have a vector potential $A(x)$ $(A: \mathbb{R}^3 \to \mathbb{R}^3)$ and electric potential $\phi(x)$ $(\phi: \mathbb{R}^3 \to \mathbb{R})$. Then, the classical Hamiltonian is

$$h(x,k) = \frac{1}{2m}|k - eA(x)|^2 + e\phi(x)$$

Quantize $\Big\}$

$$H(x,p) = \frac{1}{2m}|p - eA(x)|^2 + e\phi(x).$$

∎

$\boxed{\text{Ex}}$ (n-particle system) Say we have n particles of masses $m_1, \ldots, m_n$ and spatial coördinates $x_1, \ldots, x_n \in \mathbb{R}^3$. Moreover, translation invariance as pair interactions $V_{ij}(x_i - x_j)$ and external potentials $V_i(x_i)$.

Then, the <u>classical Hamiltonian</u> is

$$h(x,k) = \sum_{j=1}^{n} \left[\frac{1}{2m_j} |k_j|^2 + V_j(x_j) \right] + \frac{1}{2} \sum_{i \neq j} V_{ij}(x_i - x_j)$$

$x = (x_1, \ldots, x_n)$, $k = (k_1, \ldots, k_n)$.

Then, the <u>quantum Hamiltonian</u> is

$$H = \sum_{j=1}^{n} \left[\frac{1}{2m_j} |P_j|^2 + V_j(x_j) \right]$$

$$+ \frac{1}{2} \sum_{i \neq j} V_{ij}(x_i - x_j)$$

Acts on $L^2(\mathbb{R}^{3n})$

For example, consider an atom w/ infinitely heavy nucleous n electrons (w/ charge $\overset{\text{mass}=m_j}{e}$). Then, $Z = en$. So, the quantum Hamiltonian for the atom is:

$$H_{at} = \sum_{j=1}^{n} \left[\frac{1}{2m_j} |p_j|^2 - \frac{Ze}{|x_j|} \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} .$$

If the atom interacts w/ a magnetic field, then

$$H_{at}^{mag} = \sum_{j=1}^{n} \left[\frac{1}{2m_j} |p_j - Z\underset{\text{vector potential}}{A}(x_j)|^2 - \frac{Ze}{|x_j|} \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|x_i - x_j|} .$$

■

—————— // ——————

Until now, we were doing things w/out internal degrees of freedom.

* **INTERNAL DEGREES OF FREEDOM**: We assume that the states of a particle are given by a complex function $\psi : \mathbb{R}^3_x \times \mathbb{R}_t \longrightarrow \mathbb{C}$.

Quantum particles can have internal degrees of freedom. These internal d.o.f.s are described as vectors on a finitely dimensional complex inner product space V. Then, the states are represented by functions of the form $\psi : \mathbb{R}^3_x \times \mathbb{R}_t \rightarrow V$.

The state space is now:

$$L^2(\mathbb{R}^3, V) = \left\{ \psi : \mathbb{R}^3 \longrightarrow V : \int \|\psi(x)\|_V^2 \, dx < \infty \right\}.$$

Take an orthonormal basis by fcts. $V \rightarrow \mathbb{C}^m$, $m > 1$, then

$$\psi(x) = (\psi_{-r}(x), \ldots, \psi_r(x)),$$

$$r = \frac{m-1}{2}, \ m \text{ odd} \quad \text{and} \quad r = \frac{m}{2}, \ m \text{ even}.$$

$$\Rightarrow \psi_s(x) \equiv \psi(x, s)$$

spin variable

LECTURE 7

29/09/2023

STATIONARY STATES

* **STATIONARY STATES:** Consider

$$i\hbar\, \partial_t \psi = H\psi, \quad \psi(0) = \psi_0$$

where $H = H^*$ is the self-adjoint Schrödinger op.

Recall: $\boxed{\text{Gauge symmetry}} \Rightarrow \boxed{\text{(SE) has solutions.}}$

Stationary solutions:

$$\psi(x,t) = e^{i\lambda t}\phi(x), \quad \phi \in L^2(\mathbb{R}^m), \quad \lambda \in \mathbb{R}.$$

Plugging stationary solutions into (SE) shows that ϕ satisfies:

$$H\phi = \lambda\phi \quad \Rightarrow \quad (\lambda, \phi) \text{ eigenpair of } H.$$

$$\mathrm{Prob}_\psi(x \in \Omega) = \int_\Omega |\psi(x,t)|^2\, dx = \int_\Omega |\phi(x)|^2\, dx$$

Time-independent

$$\mathrm{Prob}_\psi(p \in \Omega) = \int_\Omega |\hat{\psi}(k,t)|^2 \, dk = \int_\Omega |\hat{\phi}(k)|^2 \, dk$$

NOTE: $\forall \varepsilon \ \exists R$ s.t. $\mathrm{Prob}_\psi(x \notin B_R) \leq \varepsilon$.

This follows from

$$\int_{|x| \geq R} |\phi(x)|^2 \, dx \xrightarrow{R \nearrow \infty} 0$$

$\Rightarrow$ Stationary states are called "BOUND STATES"

$\Leftrightarrow$ In stationary states, the system is in a bounded domain of $\mathbb{R}^m$.

$\Leftrightarrow$ System localized in space.

---

* SPACE-TIME LOCALIZATION OF SOLUTIONS:

Define:

$\mathcal{H}_{bnd} := \{$ span of eigenfcts of $H\}$

$$= \left\{ \phi = \sum_i c_i \varphi_i : \varphi_i \text{ eigenfcts. w/ eigenvals. } \lambda_i \right\}$$

$$\mathcal{H}_{dc} := \mathcal{H}_{bnd}^{\perp} = \{ \phi \in L^2 : \phi \perp \mathcal{H}_{bnd} \}.$$

Lemma: $\mathcal{H}_{bnd}$ and $\mathcal{H}_{dc}$ are invariant under Schrödinger evolution. More precisely, for the Schrödinger propagator U_t,

(a) $U_t(\mathcal{H}_{bnd}) = \mathcal{H}_{bnd} \quad \forall t$

(b) $U_t(\mathcal{H}_{dc}) = \mathcal{H}_{dc} \quad \forall t$.

Pf: (a) If $\psi_0 = \sum_i c_i \varphi_i$, $\{\varphi_i\}$ orthonormal basis of eigenfcts. of H. Take Fourier transform:

$$\|\psi_0\|_2^2 = \sum_i |c_i|^2 < \infty$$

$\Rightarrow$ Solution to (SE): $\psi_t(x) = \sum_j c_j e^{i\lambda_j t/\hbar} \phi_j(x)$

The above solution is <u>unique</u> b/c

$$\|\psi_t\|_2^2 = \|\psi_0\|_2^2 = \sum_j |c_j|^2 < \infty$$

conservation of probability $\Rightarrow$ uniqueness

(b) $\psi_0 \perp \mathcal{H}_{bnd} \Rightarrow \psi_t \perp \mathcal{H}_{bnd}$?

Yes! B/c U_t preserves inner products. ∎

Thm: (a) If $\psi_0 \in \mathcal{H}_{bnd}$, then $\forall \varepsilon > 0\ \exists R > 0$ s.t. $\text{Prob}_{\psi_t}(|x| > R) \leq \varepsilon \Rightarrow$ system is localized in B_R.

(b) If $\psi_0 \in \mathcal{H}_{ac}$, then $\forall R > 0$,

$$\text{Prob}_{\psi_t}(x \in B_R) \longrightarrow 0 \text{ in the } \underbrace{\text{ergodic sense}} \text{ as } t \to \infty$$

i.e., system escapes from any domain

"$f(t) \to 0$ in the ergodic sense" $\Leftrightarrow$ $\frac{1}{T}\int_0^T f(t)\,dt \to 0$ as $T \to \infty$.

(RUELLE'S THM)

Pf: (a) Suppose

$$\psi_0(x) = \sum_j c_j \varphi_j(x) \Rightarrow \psi_t(x) = \sum_j c_j e^{i\lambda_j t/\hbar} \phi_j(x)$$

Consider

$$\chi_R(x) := \begin{cases} 1, & |x| > R \\ 0, & |x| \leq R \end{cases}.$$

Then,

$$\chi_R \psi_t = \sum_{j=1}^{N} c_j e^{i\lambda_j t/\hbar} \underbrace{\chi_R \varphi_j}_{\text{Not orthonormal (almost though)}}$$

By the triangle inequality:

$$\|\chi_R \psi_t\| \leq \sum_{j=1}^{N} |c_j| \, \|\chi_R \varphi_j\|$$

$$\overset{\text{Cauchy}}{\leq} \underbrace{\left(\sum_{j=1}^{N} |c_j|^2\right)^{1/2}}_{\|\psi_0\| = 1} \left(\sum_{j=1}^{N} \|\chi_R \varphi_j\|^2\right)^{1/2}$$

$$\leq N^{1/2} \max_j \|\chi_R \varphi_j\| \leq \varepsilon .$$

R: $\|\chi_R \varphi_j\| \leq \varepsilon/\sqrt{N}$

$\blacksquare$

<u>Prop</u>: If $H = H^*$, then the eigenfcts. of H w/ different eigenvalues are orthogonal.

Pf: $\langle H\varphi_j, \varphi_i \rangle = \langle \varphi_j, H\varphi_i \rangle$. $\square$

* **SPECTRAL THEORY**: Different space-time behaviours described in terms of the spectrum of the Schrödinger operator.

Def: (INVERSE) Let A be an operator on a Hilbert space $\mathcal{H}$. Then A is <u>invertible</u> if A has a <u>bounded</u> <u>inverse</u>.

Def: (SPECTRUM) The spectrum of A is:

$$\sigma(A) := \{\lambda \in \mathbb{C} : A - \lambda \mathrm{Id} \text{ is } \underline{\underline{\text{not}}} \text{ invertible}\}$$

Properties: !!!

(i) $\sigma(A) \subset \mathcal{H}$ is closed.

(ii) A bounded $\Leftrightarrow$ $\sigma(A)$ bounded.

(iii) $A = A^*$ $\Rightarrow$ $\sigma(A) \subset \mathbb{R}$.

(iv) $A = A^*$ $\Rightarrow$ $\sigma(A) \neq \emptyset$

Def: (DISCRETE SPECTRUM)

$$\sigma_d(A) := \left\{ \lambda \in \mathbb{C} : \lambda \text{ isolated eigenval. with finite multiplicity} \right\}$$

Def: (ESSENTIAL SPECTRUM)

$$\sigma_{ess}(A) := \sigma(A) \setminus \sigma_d(A)$$

---

* **ATTAINABLE VALUES**: Let A be a self-adjoint operator on $\mathcal{H}$. Then,

$$\mathrm{Prob}_\psi(A \in \underset{\substack{\uparrow \\ I=[a,b]\subset\mathbb{R}}}{I}) = \langle \psi, \chi_I(A)\,\psi \rangle$$

where χ_I indicator fct. of $I \subset \mathbb{R}$

Then

$$\chi_I(\lambda) = C \lim_{\varepsilon \to 0} \frac{1}{2\pi} \int_I \underbrace{\frac{\varepsilon}{(\lambda-\mu)^2 + \varepsilon^2}}_{\text{Converges to } \delta(\lambda-\mu) \text{ (Dirac } \delta)} d\mu$$

Normalizing constant.

Now,

$$\delta_\varepsilon(\lambda-\mu) = \frac{1}{2\pi}\frac{\varepsilon}{(\lambda-\mu)^2+\varepsilon^2} = \frac{1}{\pi}\operatorname{Im}(\lambda-\mu-i\varepsilon)^{-1}.$$

Claim: $\delta_\varepsilon(A-\mu) = \frac{1}{\pi}\operatorname{Im}\underbrace{(A-\mu-i\varepsilon)^{-1}}_{\text{"RESOLVENT"}}$ is well-defined

Pf: $A^* = A \Rightarrow \sigma(A) \subset \mathbb{R}$

$\Rightarrow \mu + i\varepsilon \notin \sigma(A) \quad \forall \mu \in \mathbb{R}$

$\Rightarrow A-\mu-i\varepsilon$ has bounded inverse, hence is invertible.

So, we define:

$$\chi_I(A) := \lim_{\varepsilon\to 0}\int_I \delta_\varepsilon(A-\mu)\, d\mu.$$

In which sense?

Unif.: $\| \chi_I^{(\varepsilon)}(A) - \chi_I(A) \| \to 0$ Definitely not

Strong: $\| \chi_I^{(\varepsilon)}(A)\psi - \chi_I(A)\psi \| \to 0$

Weak: $| \langle \phi, (\chi_I^{(\varepsilon)}(A) - \chi_I(A))\psi \rangle | \to 0$

as $\varepsilon \to 0$ $\forall \phi, \psi \in L^2$.

!

Upshot: All possible measured values of the observable A in any state ψ lie in the spectrum of A, $\underbrace{\sigma(A) \subset \mathbb{R}}_{A = A^*}$.

Def: (ATTAINABLE VALUE) λ is an attainable value of A in state ψ if and only if

$$\mathrm{Prob}_\psi(A \in I) \neq 0 \quad \forall I \ni \lambda.$$

Def: (RESOLVENT) The resolvent set of A is

$$\rho(A) := \mathbb{C} \setminus \sigma(A)$$

!

IMPORTANT

Prop: λ is an attainable value for A at least for some state ψ if and only if $\lambda \in \sigma(A)$

Pf: ($\Rightarrow$) If λ is attainable, then $\rho(A) = \mathbb{C} \setminus \sigma(A)$ is <u>not</u> attainable. This is equivalent to

$$\{\text{attainable value}\} \cap \rho(A) = \emptyset .$$

So, let $I \subset \rho(A) \cap \mathbb{R}$. Then

$$\mathrm{Prob}_\psi (A \subset I)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\pi} \left\langle \psi, \int_I \mathrm{Im}(A - \mu - i\varepsilon)^{-1} \psi \, d\mu \right\rangle$$

$\mu \in \sigma(A)$

$$\overset{\downarrow}{=} \frac{1}{\pi} \left\langle \psi, \int_I \underbrace{\mathrm{Im}\,(A-\mu)^{-1}}\psi \, d\mu \right\rangle$$

$$\mathrm{Im}(A-\mu)^{-1} = \frac{1}{2i}\left[(A-\mu)^{-1} - (A-\mu)^{-1*}\right]$$

These two are equal.

$$= 0 .$$

since $A = A^*$

∎

LECTURE 8

06/10/2023

DISCRETE & ESSENTIAL SPECTRUM

Recall: The spectrum of an operator A is

$$\sigma(A) := \{ \lambda \in \mathbb{C} : A - \lambda \, \mathrm{Id} \text{ is } \underline{\text{not}} \text{ invertible} \}$$

Now,

$\boxed{B \text{ invertible}} \iff \boxed{B \text{ has a bounded inverse}}$

$\iff \boxed{\ker B = \{0\} \text{ and } \operatorname{im} B = \mathcal{H}}$

! **WARNING**: B is not invertible if either

- $\ker B \neq \{0\}$ ($\iff$ 0 eigenvalue of B)
- or $\operatorname{im} B \subsetneq \mathcal{H}$ (i.e., B has inverse on $\operatorname{im} B$

but B^{-1} is <u>not</u> bounded).

- or both

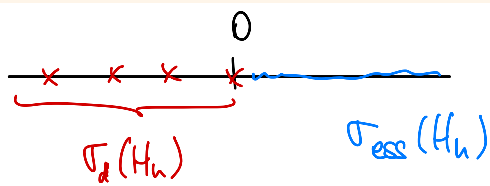
"pure point" complex numbers

Defin: (i) $\sigma_{pp}(A) = \{ \text{all eigenvals. of } A \}$

(ii) $$\sigma_d(A) = \left\{ \lambda \in \sigma(A) : \begin{array}{l} \lambda \text{ isolated and} \\ \text{finite multiplicity} \end{array} \right\}$$

- The eigenval. λ of A is isolated iff $\exists$ neighborhood $U \ni \lambda$ s.t. $U \cap \sigma(A) = \{\lambda\}$.
- Multiplicity of λ = $\dim \ker(A - \lambda)$

(iii) $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A)$.



Ex: Orthogonal projection P (i.e., $P^2 = \mathrm{Id}$ and $P^* = P$) of finite rank. Then

$$\sigma(P) = \{0, 1\}, \quad \sigma_d(P) = \{1\},$$

$$\sigma_{ess}(P) = \{0\}, \quad \sigma_{pp}(P) = \sigma(P)$$

$\blacksquare$

Define the spaces:

(i) $\mathcal{H}_{pp} := \text{span}\{\text{eigenfcts. of } A\}$

(ii) $\mathcal{H}_{disc} := \text{span}\{\text{eigenfcts. of } A \text{ corresp. to } \sigma_d(A)\}$

(iii) $\mathcal{H}_{ess} := \mathcal{H}_{disc}^{\perp}$.

Decaying states $\leftrightsquigarrow$ Essential spectrum.

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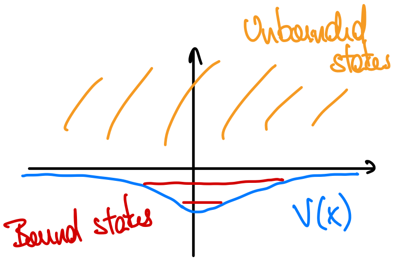
* **SPECTRA OF SCHRÖDINGER OPERATORS**:

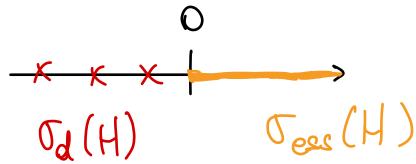
Consider the Schrödinger operator given by

$$H = -\frac{\hbar^2}{2m}\Delta + V(x)$$

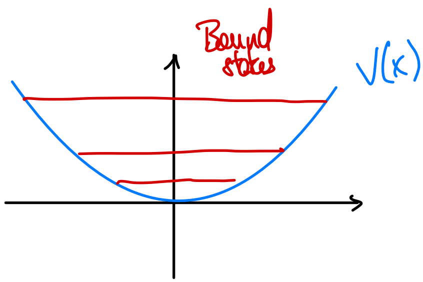
(i) If $V(x) \to 0$ as $|x| \to \infty$ (and, say $V \in L^2(\mathbb{R}^3)$), then $\sigma_{ess}(H) = [0, \infty)$



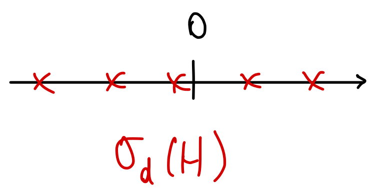
$\rightsquigarrow$



(ii) If $V(x) \to \infty$ as $|x| \to \infty$, then $\sigma_{ess}(H) = \{\infty\}$



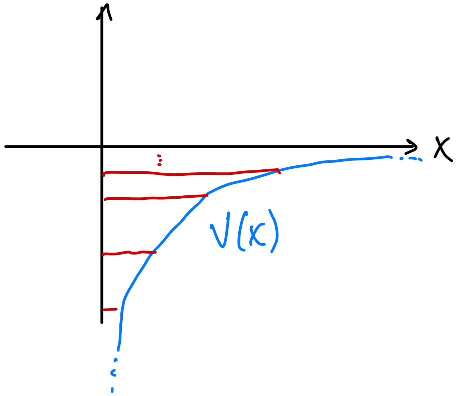
$\rightsquigarrow$

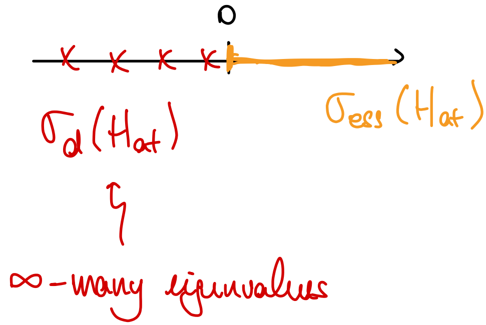


<u>EXAMPLE</u>: HYDROGEN ATOM The Schrödinger op. is

$$H_{at} = -\frac{\hbar^2}{2m}\Delta \underbrace{- \frac{\alpha}{|x|}}_{\text{Coulomb potential}}$$

Then, $V(x) \to 0$ as $|x| \to \infty$, so





"Balmer series"

Frequencies absorbed/emitted $\rightsquigarrow \hbar\omega = E_n - E_m$

$$= R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

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* **MANY-PARTICLE QUANTUM SYSTEMS**: Consider a system of n particles of masses $m_1, \ldots, m_n$ and interacting via 2-body potentials $W_{ij}(x_i - x_j)$. Moreover, suppose there is an external potential given by $V_j(x_j)$. Then, the Schrödinger operator is:

$$H_n = \sum_{k=1}^{n} \left[-\frac{\hbar^2}{2m_k} \Delta_{x_k} + V_k(x_k) \right] + \frac{1}{2} \sum_{i \neq j} W_{ij}(x_i - x_j)$$

on $L^2(\mathbb{R}^{3n}, \mathbb{C}^{9n})$, $\mathbb{R}^{3n} = \{(x_1, \ldots, x_n) : x_i \in \mathbb{R}^3\}$.

* **IDENTICAL PARTICLES**: Suppose all particles are identical (i.e., same masses, spins, interactions, etc.). Then

$$H_n = \sum_{k=1}^{n} \left[-\frac{\hbar^2}{2m} \Delta_{x_k} + V_k(x_k) \right] + \frac{1}{2} \sum_{i \neq j} W_{ij}(x_i - x_j)$$

acting on $L^2\left((\mathbb{R}^3 \times \Sigma_q)^n, \mathbb{C} \right)$, where

$$\Sigma_q := \{ -r, \_\_\_, r \}, \quad r = \begin{cases} q/2, & q \text{ even} \\ \frac{q-1}{2}, & q \text{ odd} \end{cases}$$

spin $s \in \Sigma_q$

FACT: All particles are either fermions or bosons.

$$\mathcal{H}_{fermi} := \left\{ \psi \in L^2\left((\mathbb{R}^3 \times \Sigma_q)^n, \mathbb{C} \right) : \psi \text{ odd under permutation of two parts} \right\}$$

$$\mathcal{H}_{bos} := \left\{ \psi \in L^2\left((\mathbb{R}^3 \times \Sigma_q)^n, \mathbb{C} \right) : \psi \text{ even under permutation of two parts} \right\}$$

Claim: $L^2\left((\mathbb{R}^3 \times \Sigma_q)^n, \mathbb{C} \right) \neq \mathcal{H}_{fermi} \oplus \mathcal{H}_{bos}$ in general

Def: Let S_n be the symmetric group; i.e., the group of permutations of n indices. For $\pi \in S_n$,

$$(1, \ldots, n) \xmapsto{\pi} (\pi(1), \ldots, \pi(n)).$$

So, if $\pi \in S_n$, then it maps

$$(z_1, \ldots, z_n) \xmapsto{\pi} (z_{\pi(1)}, \ldots, z_{\pi(n)}).$$

Def: Representation of S_n on $L^2((\mathbb{R}^3 \times \Sigma_q)^n)$ is a map

$$S_n \ni \pi \longmapsto T_\pi \longleftarrow \text{operator on } L^2((\mathbb{R}^3 \times \Sigma_q)^n)$$

where

$$T_\pi[\psi](z_1, \ldots, z_n) := \psi(z_{\pi^{-1}(1)}, \ldots, z_{\pi^{-1}(n)}).$$

Then, for $z = (z_1, \ldots, z_n)$, $\pi z = (z_{\pi(1)}, \ldots, z_{\pi(n)})$ and $(T_\pi \psi)(\pi^{-1} z)$ is the representation.

The representation of S_n satisfies $T_\pi T_{\pi'} = T_{\pi\pi'}$.

$T_\pi T_{\pi'} \psi(z) = T_\pi \psi(\pi'^{-1} z) = \psi(\pi'^{-1} \pi z)$
$= \psi((\pi\pi')^{-1} z) = T_{\pi\pi'}$

So, with this, define

$$\mathcal{H}_{fermi} := \left\{ \psi \in L^2((\mathbb{R}^3 \times \Sigma_q)^n) : T_\pi \psi = (-1)^{\#(\pi)} \psi \right\}$$

$$\mathcal{H}_{bos} := \left\{ \psi \in L^2((\mathbb{R}^3 \times \Sigma_q)^n) : T_\pi \psi = \psi \right\}$$

$\#(\pi) = \#$ of crossings ("signature of π")

Claim: The Schrödinger operator of n-identical particles H_n commutes with T_π iff permutation is symmetric; i.e.,

$$\boxed{[H_n, T_\pi] = 0} \iff \boxed{\text{Permutation of identical particles is a symmetry of } H_n}$$

FACT: $\mathcal{H}_{fermi}$ & $\mathcal{H}_{bos}$ are invariant subspaces under H

FACT: In QM, interactions (and thus Schrödinger operators) are independent of spin. That is, for

$$H_n \psi(x_1, s_1, \ldots, x_n, s_n)$$

$$= \sum_{k=1}^{n} \left[-\frac{\hbar^2}{2m} \Delta_{x_k} + V(x_k) \right] \psi(x_1, \ldots, s_n)$$

$$+ \frac{1}{2} \sum_{i \neq j} W_{ij}(x_i - x_j) \psi(x_1, \ldots, s_n)$$

we can SEPARATE VARIABLES:

$$\psi(x_1, s_1, \ldots, x_n, s_n) = \phi(x_1, \ldots, x_n) \chi(s_1, \ldots, s_n)$$

↪ This gives (SE) for ϕ.

→ What permutation properties of ϕ imply that $\exists \chi$ such that $\phi \chi \in \mathcal{H}_{fermi}$?

A: Weyl of representation of S_n.

SIMPLE CASE: consider the spin 0 case; i.e.,

$$q = 1 \quad \text{and} \quad \underbrace{r}_{\text{VALUE OF THE SPIN}} = \frac{q-1}{2} = 0$$

(e.g. electrons $\rightsquigarrow r = 1/2$
$\Rightarrow q = 2r+1 = 2 \rightsquigarrow$ up and down)

ϕ antisymmetric: $\quad T_\pi \phi = (-1)^{\#(\pi)} \phi \quad \forall \pi \in S_n$.

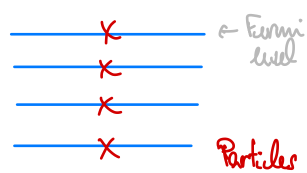
Upshot: For n identical particles, the state space is $L^2_{\text{antisymmetric}}(\mathbb{R}^3)$ (i.e., L^2 functions that are antisymmetric).

EXAMPLE: Consider the n-particle functions build out of 1-particle ones. Then

$$L^2_{sym}(\mathbb{R}^{3n}) \ni \phi(x_1) \dots \phi(x_n)$$

BOSE-EINSTEIN CONDENSATE

$$L^2_{antisym}(\mathbb{R}^{3n}) \ni \phi_1 \wedge \dots \wedge \phi_n$$



Thus: $\boxed{\phi_1 \wedge \cdots \wedge \phi_n = \det\left(\phi_i(x_j)\right)}$

STATE DETERMINANT

LECTURE 9

11/10/2023

QUANTUM MULTIPARTICLE SYSTEMS (EXAMPLES)

* **IDEAL GAS**: "Ideal" here means that there are <u>no</u> <u>interparticle</u> interactions. In a quantum gas, particles are assumed identical. So, the Hamiltonian for the system is

$$H_{igas} = \sum_{j=1}^{n} \left(-\frac{\hbar^2}{2m} \Delta_{x_j} + V(x_j) \right)$$

acting on either $\mathcal{H}_{fermi}$ or $\mathcal{H}_{bose}$ depending on whether the particles are fermions or bosons.

group of permi.

RECALL: $\mathcal{H}_{bose} = \{ \psi \in L^2(\mathbb{R}^{3n}) : T_\pi \psi = \psi \ \forall \pi \in S_n \}$

spinless fermions $\to$ $\mathcal{H}_{fermi} = \{ \psi \in L^2(\mathbb{R}^{3n}) : T_\pi \psi = (-1)^{\#(\pi)} \psi \ \forall \pi \in S_n \}$

Parity of π = # transpositions

$$= \underbrace{L^2(\mathbb{R}^3) \wedge \dots \wedge L^2(\mathbb{R}^3)}_{n \text{ times}}$$

$$= \underbrace{P_{anti}}_{} \left(L^2(\mathbb{R}^3) \otimes \dots \otimes L^2(\mathbb{R}^3) \right)$$

Antisymmetrization operator:

$$P_{anti} = \frac{1}{n!} \sum_{\pi \in S_n} (-1)^{\#(\pi)} T_\pi$$

orthogonal projection
$P^* = P$ $\quad$ $P^2 = P$

PROBLEM: Find the eigenvalues of H_{gas}.

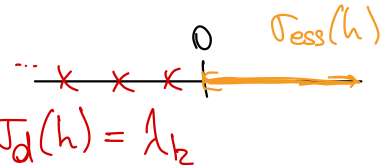
PARTIAL SOLUTION: The eigenvalues of H_{gas} on $L^2(\mathbb{R}^{3n})$ are:

$$\left\{ \sum_{j=1}^{n} \lambda_{k_j} : \lambda_k \text{ eigenvalues of } h \right\},$$

$$h = -\frac{\hbar^2}{2m}\Delta_x + V(x) \text{ on } L^2(\mathbb{R}^3)$$

Now, if $V \to 0$ as $|x| \to \infty$, then

Unbound states $\longrightarrow$ $\sigma_{ess}(h) = [0, \infty)$



Note that $h\phi_k = \lambda_k \phi_k$ and $H_{gas} = \sum_{j=1}^{n} h_j$.

Def: (GROUND STATE) The ground state is the eigenfunction corresponding to the smallest eigenvalue.

In this sense, the ground state of H_{gas} on $L^2(\mathbb{R}^{3n})$ is $\prod_{j=1}^{n} \phi_1(x_j) \in \mathcal{H}_{bose}$ and the ground state energy is $E_1 = n\lambda_1$, where λ_1 is the eigenvalue corresponding to ϕ_1. So,

- Ground state of H_{gas} on $\mathcal{H}_{bose}$ $\rightsquigarrow \prod_{j=1}^{n} \phi_1(x_j)$
- Ground state energy of H_{gas} on $\mathcal{H}_{bose}$ $\rightsquigarrow n\lambda_1$

On $\mathcal{H}_{fermi}$, the eigenfunctions of H_{gas} are

$$\left\{ \phi_{k_1} \wedge \cdots \wedge \phi_{k_n} : h\phi_k = \lambda_k \phi_k \right\}$$

$\Rightarrow$ All ϕ_{k_j} must be distinct and mutually orthogonal

If $\phi_2 = c\phi_1 + \phi_1^\perp$, $\langle \phi_1, \phi_1^\perp \rangle = 0$, then

$$\phi_1 \wedge \phi_2 = \cancel{\phi_1 \wedge c\phi_1}^{\,0} + \phi_1 \wedge \phi_1^\perp = \phi_1 \wedge \phi_1^\perp$$

$$\bigwedge_{j=1}^{n} f_j = \bigwedge_{j=1}^{n} f_j^\perp$$

$\Rightarrow$ Can take $\{\phi_{k_j}\}$ to be an orthonormal basis.

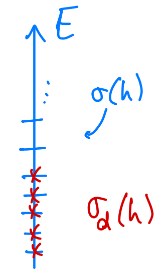
Thus,

- Ground state of H_{gas} on $\mathcal{H}_{fermi}$ $\rightsquigarrow \displaystyle\bigwedge_{j=1}^{n} \phi_j(x_j)$

- Ground state energy of H_{gas} on $\mathcal{H}_{fermi}$ $\rightsquigarrow \displaystyle\sum_{j=1}^{n} \lambda_j$

Denote by $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ the n first eigenvals of h (repeated according to multiplicity). For a bosonic atom w/ n electrons, ground state energy is $n\lambda_1$.

But, for fermions, it is $\sum_{j=1}^{n} \lambda_j$



$$h = -\frac{\hbar^2}{2m}\Delta_x - \frac{\alpha Z e^2}{|x|}$$

$Z = n \rightsquigarrow$ charge $= Ze$

$\Longrightarrow$ Eigenvalues of h are $\lambda_k = \dfrac{-c(eZ)^4}{k^2}$

constant

Obs:

$$E_{bose} = -ce^4 n^5$$

$\Downarrow \leftarrow$ for a fixed n

$$E_{fermi} = \sum_{k=1}^{n} \frac{-c(en)^4}{k^2}.$$

$\blacksquare$

LECTURE 10 — QUANTUM STATISTICS

13/10/2023

Assuming we know that the system is in the state ψ_j with probability $P_j > 0$.

There are 2 types of uncertainties:

- <u>Extrinsic</u> : $j = 1, \ldots, n$
- <u>Intrinsic</u> : ψ_j.

Now, we want to compute the expectation value of an observable A on this state ψ_j :

$$\mathrm{Av}_{\psi_j}(A) = \langle A \rangle_{\psi_j} := \langle \psi_j , A \psi_j \rangle .$$

Say that the probability of being in ψ_j is P_j.

Define

$$\langle A \rangle := \sum_{j=1}^{n} P_j \langle A \rangle_{\psi_j} , \quad P_j > 0, \ \sum_{j=1}^{n} P_j = 1$$

Compare this w/ the average in

$$\psi := \sum_{j=1}^{n} a_j \psi_j .$$

QM interprets the probability of finding system in ψ_j as $|a_j|^2$. Then

$$\langle A \rangle_\psi \overset{\text{def}}{=} \sum_{i,j} \langle \psi_i, A \psi_j \rangle \neq \langle A \rangle \text{ unless}$$

$$\langle \psi_i, A\psi_j \rangle \neq 0 \ \forall i \neq j.$$

So, we need to redefine some things:

$$\langle A \rangle_\psi := \operatorname{tr}(AP_\psi),$$

where P_ψ is the rank-one orthogonal projection onto ψ.

$$\|\psi\| = 1 \Rightarrow P_\psi f = \psi \langle \psi, f \rangle$$

$$\Leftrightarrow P_\psi = |\psi\rangle\langle\psi|$$

where the ridiculous bra $\langle \psi|$ is a functional $\langle\psi| : f \mapsto \langle \psi, f\rangle$ and $|\psi\rangle : z \mapsto z\psi$.

Properties defining trace:

(i) $\operatorname{tr}(\mathrm{Id}) = 1$

(ii) $\operatorname{tr}(AB) = \operatorname{tr}(BA)$

(iii) $\operatorname{tr}(\alpha A + \beta B) = \alpha \operatorname{tr}(A) + \beta \operatorname{tr}(B)$

These uniquely define the trace map

$$\boxed{S \text{ is "trace class"}} \iff \boxed{\operatorname{tr}|S| < \infty, \text{ where } |S| = \sqrt{S^* S}}$$

In general,

$$\operatorname{tr} \rho = \sum_j \langle f_j, \rho f_j \rangle, \quad \{f_j\} \text{ orthonormal basis}$$

Ex: $\operatorname{tr} P_\psi = \|\psi\|^2$.

Def: (POSITIVE OPERATOR)

$$\boxed{A \text{ is non-negative } (A \geq 0)} \iff \boxed{\langle f, Af \rangle \geq 0 \quad \forall f \in \mathcal{H}}$$

Obs: $\langle A \rangle = \operatorname{tr}(A\rho), \quad \rho = \sum_{j=1}^n p_j P_{\psi_j}$. Indeed,

$$\operatorname{tr}(A\rho) = \sum p_j \operatorname{tr}(A P_{\psi_j}) = \sum p_j \langle \psi_j, A\psi_j \rangle = \langle A \rangle$$

$$\mathrm{tr}(AP_\psi) = \langle \psi, A\psi \rangle .$$

Obs: Properties of the operator

$$\rho := \sum_j p_j P_{\psi_j} , \quad \{\psi_j\} \text{ orthonormal basis :}$$

- $\rho \geq 0$
- $\mathrm{tr}\, \rho = \sum_j p_j = 1$

Operators w/ these properties are called DENSITY OPERATORS

$\Rightarrow$ Expand the state space from $\mathcal{H}$ to S_1^+, the space of positive trace class operators

$$S_p = \{ \gamma \text{ operator on } \mathcal{H} : \mathrm{tr}|\gamma|^p < \infty \}$$

"SCHATTEN SPACE" (expands the notion of state)

Expand the notion of average: the average of an observable A (which is an operator on $\mathcal{H}$) in state ρ is

$$\boxed{Av_\rho(A) := tr(A\rho)}$$

Dynamics: Assume $\{\psi_j\}$ satisfies (SE)

$$i\hbar\partial_t \psi = H\psi,$$

where $\{\psi_j|_{t=0}\}$ forms an orthonormal basis. This means that $\{\psi_j\}$ is an orthonormal basis for all time. Then,

$$\boxed{\rho = \sum_j p_j P_{\psi_j}} \quad \text{satisfies} \quad \boxed{\partial_t \rho = -\frac{i}{\hbar}[H,\rho]}$$

VON NEUMANN (or Landau) EQUATION

Determines the dynamics / evolution of the state $\rho \in S_1^+$.

Upshot: Dynamics of density operators is given by the von Neumann equation.

This framework of

$$\left(S_1^+,\ Av.(\cdot),\ \text{von Neumann Equation}\right)$$

is called **QUANTUM STATISTICS**

This makes "usual" QM a special case of Quantum Statistics (QS):

ψ satisfies (SE) $\overset{\text{HN}}{\Longleftrightarrow}$ Rank-one projection satisfies von Neumann eq.

Obs: Can define the Hilbert-Schmidt inner product $\langle S, T\rangle := \operatorname{tr}(S^* T)$.

Induces norm: $\|T\|_{S_p} := \left(\operatorname{tr}(|T|^p)\right)^{1/p}$.

"Just like Lebesgue spaces"

* **INFORMATION REDUCTION**: Consider a compound system (T) consisting of several subsystems (each of them being a Hilbert space). That is, for only 2 subsystems, S and E, we have their (Hilbert) state spaces $\mathcal{H}_S$ and $\mathcal{H}_E$, respectively. Then,

$$\mathcal{H}_T = \mathcal{H}_S \otimes \mathcal{H}_E .$$

compound system

Obs:

$$X \otimes Y = \text{span}\left\{ f_j \otimes g_i : \begin{array}{l} \{f_j\} \text{ orthonor. basis of } X \\ \{g_i\} \text{ orthonor. basis of } Y \end{array} \right\}$$

Ex: $L^2(dx) \otimes L^2(dy) = L^2(dx \otimes dy)$.

Given a compound system $T = SE$ and a state $\psi \in \mathcal{H}_T = \mathcal{H}_S \otimes \mathcal{H}_E$, assume we are interested in measuring an observable only of S on $\mathcal{H}_S$.

Q: Can we do this?

A: Extend the observable A acting on $\mathcal{H}_S$ to an observable on $\mathcal{H}_S \otimes \mathcal{H}_E$ by setting it to be $A \otimes \mathrm{Id}_E$.

QUESTION: Given $\psi \in \mathcal{H}_T$, is there a $\phi \in \mathcal{H}_S$ such that

$$\langle \psi, A\psi \rangle = \langle \phi, A\phi \rangle$$

for all operators A acting on $\mathcal{H}_S$?

ANSWER: The above holds iff $\psi = \phi \otimes x$ for some $x \in \mathcal{H}_E$ (i.e., S and E are <u>not</u> correlated).

Pf: Check for $\psi = \alpha_1 \phi_1 \otimes x_1 + \alpha_2 \phi_2 \otimes x_2$

QUESTION: Can we extend the state space so that the above holds regardless of the correlation between S and E?

ANSWER: Yes! Smallest such space is the <u>space of density operators</u>.

Lecture 11 — Compound Quantum Systems

18/10/2023

Compound system: System C composed of several quantum subsystems A_j, $j = 1, \dots, n$:

$$C = A_1 \otimes A_2 \otimes \cdots \otimes A_n$$

⇝ Bipartide compound system $(n=2)$: $C = A \otimes B$

Ex: An n particle system can be broken into a system w/ k particles and another one w/ $n-k$ partic.

Ex: Atom + Environment (small system) We have that the state space of the compound bipartide system is

$$C = A \otimes B \rightsquigarrow \mathcal{H}_C = \mathcal{H}_{AB} = \underbrace{\mathcal{H}_A}_{\text{state space of } A} \otimes \underbrace{\mathcal{H}_B}_{\text{state space of } B}$$

More precisely:

Def: Let $\{e_i^A\}$ be an orthonormal basis for $\mathcal{H}_A$ and let $\{e_j^B\}$ be an orthonormal basis for $\mathcal{H}_B$.

Then,

$$\boxed{\mathcal{H}_A \otimes \mathcal{H}_B = \left\{ \sum_{i,j} c_{ij}\, e_i^A \otimes e_j^B : \sum_{i,j} |c_{ij}|^2 < \infty \right\}}$$

Independent of choice of basis.

Def: Inner product on $\mathcal{H}_A \otimes \mathcal{H}_B$ is defined as: for $\phi \in \mathcal{H}_A$ and $\psi \in \mathcal{H}_B$, then

$$\phi \otimes \psi := \sum_{i,j} a_i b_j\, e_i^A \otimes e_j^B$$

and

$$\boxed{\langle \tilde{\phi} \otimes \tilde{\psi}, \phi \otimes \psi \rangle_{\mathcal{H}_{AB}} := \langle \tilde{\phi}, \phi \rangle_{\mathcal{H}_A} \langle \tilde{\psi}, \psi \rangle_{\mathcal{H}_B}}.$$

Extend by linearity

Def: The subsystems A and B are said to be <u>correlated</u> in a state ψ_{AB} iff

$$\psi_{AB} \neq \psi_A \otimes \psi_B \quad \forall \psi_A \in \mathcal{H}_A, \ \forall \psi_B \in \mathcal{H}_B$$

$$\Longleftrightarrow \quad c_{ij} \neq a_i b_j \quad \forall \{a_i\}, \ \forall \{b_j\}.$$

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* <u>INFORMATION / STATE REDUCTION</u>

Consider a bipartite system $T = SE$. Suppose we don't know anything about E (or, equivalently, aren't interested in info. about E).

We <u>only</u> want to measure properties about S.

<u>QUESTION</u>: Given ψ_{SE}, is there ψ_S such that

$$\langle \psi_{SE}, \underbrace{A}_{} \psi_{SE} \rangle_{\mathcal{H}_{SE}} \overset{(*)}{=} \langle \psi_S, A \psi_S \rangle_{\mathcal{H}_S} \quad \forall \text{ observable } A \text{ acting on } \mathcal{H}_S \ ?$$

It is actually $A \otimes \mathrm{Id}_{\mathcal{H}_E}$ since A acts only on $\mathcal{H}_S$

Prop: $(*)$ holds (i.e., answer to above question is "yes")

$\iff$ S and E are <u>not</u> correlated in ψ_{SE}.

$\iff$ $\psi_{SE} = \psi_S \otimes \psi_E$ for some $\psi_S \in \mathcal{H}_S$ and $\psi_E \in \mathcal{H}_E$

Pf: $(\Leftarrow)$ If we can write

$$\psi_{SE} = \psi_S \otimes \psi_E \text{ for some } \psi_S \in \mathcal{H}_S, \ \psi_E \in \mathcal{H}_E$$

then

$$\begin{aligned}
\langle \psi_{SE}, A\psi_{SE} \rangle_{SE} &= \langle \psi_S \otimes \psi_E, (A\psi_S) \otimes \psi_E \rangle_{SE} \\
&= \langle \psi_S, A\psi_S \rangle_S \underbrace{\langle \psi_E, \psi_E \rangle_E}_{=1} \\
&= \langle \psi_S, A\psi_S \rangle_S .
\end{aligned}$$

$(\Rightarrow)$ Conversely, suppose $(*)$ holds. Then, <u>first</u>, take the simplest correlated state:

$$\psi_{SE} = \frac{1}{\sqrt{2}} \left(\phi_1 \otimes \psi_1 + \phi_2 \otimes \psi_2 \right)$$

where $\langle \phi_1, \phi_2 \rangle_S = \langle \psi_1, \psi_2 \rangle_E = 0$. Consider a state ξ s.t. $\xi \perp \psi_S$ (i.e., $\langle \xi, \psi_S \rangle_S = 0$) by contradiction

Let $A = P_\xi$ (ortho. projec. onto ξ). Then

$$\langle \psi_S, P_\xi \psi_S \rangle_S = | \langle \psi_S, \xi \rangle |^2 = 0$$

On the other hand,

$$\langle \psi_{SE}, P_\xi \psi_{SE} \rangle_{SE} = \frac{1}{2} \Big(\phi_1 \otimes \psi_1 + \phi_2 \otimes \psi_2 ,$$

$$(P_\xi \phi_1) \otimes \psi_1 + (P_\xi \phi_2) \otimes \psi_2 \Big\rangle$$

$$= \frac{1}{2} \left(\langle \phi_1, P_\xi \phi_1 \rangle + \langle \phi_2, P_\xi \phi_2 \rangle \right)$$

$$= \frac{1}{2} \left(|\langle \phi_1, \xi \rangle|^2 + |\langle \phi_2, \xi \rangle|^2 \right)$$

Can choose ξ such that this is $\neq 0$

$$\neq 0$$

Either $\psi_S \neq \phi_1, \phi_2 \Rightarrow$ Take $\xi \perp \psi_S$ and $\xi \not\perp \phi_1$.

or $\psi_S = \phi_1 \Rightarrow$ Take $\xi = \phi_2$

or $\psi_S = \phi_2 \Rightarrow$ Take $\xi = \phi_1$

Then LHS(*) $\neq 0$ but RHS(*) $= 0$

$\hookrightarrow // \hookleftarrow$

Provisional. Need to do for the general case w/ Gram-Schmidt.

<u>Upshot</u>: • We cannot ignore information about E and stay in $\mathcal{H}_S$.

$\Rightarrow$ Have to expand the state space (i.e., extend this QM framework).

Want to compute $\langle \psi_{SE}, A\psi_{SE} \rangle_{SE}$ (#) for all observable A acting on $\mathcal{H}_S$.

Let $\{\chi_i^E\}$ be an orthonormal basis in $\mathcal{H}_E$. Use completeness relation: $\sum_i |\chi_i^E\rangle\langle\chi_i^E| = \mathrm{Id}$ (##)

$$\Updownarrow$$

$$f = \sum_i |x_i^E\rangle\langle x_i^E | f\rangle$$

$$= \sum_i \langle x_i, f\rangle_E \, x_i$$

Use (##) into (#) and use that A doesn't act on x_i^E to show that

$$\langle \psi_{SE}, A\psi_{SE}\rangle_{SE} = tr_S(A\rho_{\psi_{SE}}) \quad , \quad \text{where}$$

$$\rho_{\psi_{SE}} := \sum_i |\phi_i\rangle\langle\phi_i| \, , \quad \phi_i := \langle x_i^E, \psi_{SE}\rangle$$

So, $\forall \phi_i \in \mathcal{H}_S$, $\langle f, \phi_i\rangle_S \overset{(**)}{=} \langle \underbrace{f \otimes x_i^E}_{\in\, \mathcal{H}_{SE}}, \underbrace{\psi_{SE}}_{\in\, \mathcal{H}_{SE}} \rangle_E$

$\Rightarrow \forall f \in \mathcal{H}_S$, ϕ_i is defined by $(**)$

LECTURE 12 — INFORMATION REDUCTION

20/10/2023

GOAL: Given a wavefct. ψ of total system $T = SE$, we want to describe properties of S in its own terms without appealing to ψ in other frames (usually we don't know ψ at all).

LAST TIME: $\psi \in \mathcal{H}_{SE} \not\Rightarrow \exists \phi \in \mathcal{H}_S$ s.t. $\forall A$ acting on $\mathcal{H}_S$, $\langle \psi, A\psi \rangle_{SE} = \langle \phi, A\phi \rangle_S$

That is, in general, $\nexists \phi \in \mathcal{H}_S$ s.t. $\psi = \phi \otimes x$ for $x \in \mathcal{H}_E$.

Obs: $A\psi \equiv (A \otimes Id_{\mathcal{H}_E})\psi = (A\phi) \otimes x$.

$\Rightarrow$ Have to extend state space $\mathcal{H}_S$ of S so that:

(i) $\forall \psi \in \mathcal{H}_{SE}$ there exists a density operator ρ_ψ on S such that

$$\langle \psi, A\psi \rangle = tr_S(A\rho_\psi),$$

where $tr_S(\cdot)$ = trace of operators acting on $\mathcal{H}_S$.

QUESTION: What about density operators on the total extended state space of $T = SE$?

Claim: For all density operators R on the total space, there exists a density operator ρ_R on S s.t.

$$tr_T(AR) = tr_S(A\rho_R) \qquad (*)$$

Given $(*)$, we can forget about R and work w/ S density operators ρ acting on $\mathcal{H}_S$ only.

Pf: Using $\langle \psi, A\psi \rangle = tr_S(AP_\psi)$, with the fact that

$\psi \leftrightarrow P_\psi$

$$\forall \psi \in \mathcal{H}_{SE} \; \exists \rho_\psi \text{ on } S \text{ s.t. } \langle \psi, A\psi \rangle \overset{(\#)}{=} tr_S(A\rho_\psi)$$

we find that

$$\underset{(\#\#)}{tr_S(AP_\psi) = tr_S(A\rho_{P_\psi})}, \quad \text{where } \rho_{P_\psi} = \rho_\psi$$

Spectral decomposition:

$$R = \sum_i r_i P_{\psi_i} , \quad R\psi_i = r_i \psi_i \quad (*)$$

Why can we do this?

<u>Thm</u>: Any trace class, self-adjoint op. R can be written as $R = \sum_i r_i P_{\psi_i}$ with $r_i \in \mathbb{R}$ s.t.

$$\sum_i |r_i| = \operatorname{tr}|R| < \infty$$

Pf: Min-max argument. Take it for granted

Then, by $(*)$ we can write

$$\operatorname{tr}(AR) = \sum_i r_i \operatorname{tr}(AP_{\psi_i})$$

$$(1)$$

$$\overset{(\#\#)}{=} \sum_i r_i \operatorname{tr}(A\rho_{\psi_i})$$

Consider $\rho_{\psi_i} \overset{(2)}{=} \sum_i p_{ij} P_{\phi_{ij}}$, where $\rho_{\psi_i} \phi_{ij} = p_{ij} \phi_{ij}$

Thus, by (1) and (2),

$$\mathrm{tr}(AR) = \mathrm{tr}_S\Big(A \underbrace{\sum_{ij} r_i P_{ij} P\phi_{ij}}_{=:\,\rho_R}\Big).$$

Therefore, for a given R density op. on SE, there is a density op. ρ_R on S such that

$$\mathrm{tr}_T(AR) = \mathrm{tr}_S(A\rho_R), \text{ as desired.} \qquad \blacksquare$$

UPSHOT: Information reduction from density op. on $T = SE$ to a density op. on S by

$$\underbrace{\mathrm{tr}^E}_{\text{Partial trace}} : SE\text{-density op.} \rightsquigarrow S\text{-density op } \rho_R$$

Thus, we can rewrite $\mathrm{tr}_T(AR) = \mathrm{tr}_S(A\rho_R)$ as:

$$\boxed{\mathrm{tr}(AR) = \mathrm{tr}_S(A\underbrace{\mathrm{tr}^E R}_{\text{density op. on } S})}$$

* PROPERTIES OF PARTIAL TRACE:

$$\mathrm{tr}^E : \left\{ \begin{array}{c} \text{operators on} \\ \mathcal{H}_{SE} \end{array} \right\} \longrightarrow \left\{ \begin{array}{c} \text{operators on} \\ \mathcal{H}_S \end{array} \right\}$$

Ex:
$$\mathrm{tr}^E \begin{pmatrix} a & b & c & d \\ e & f & g & h \\ i & j & k & l \\ m & n & o & p \end{pmatrix} = \begin{pmatrix} a+f & c+h \\ i+n & k+p \end{pmatrix}$$

(a) LINEAR

(b) POSITIVE

(c) $\mathrm{tr}^E(BR) = B\,\mathrm{tr}^E R \quad \forall B$ op. on S.

Prop: For any orthonormal basis $\{x_i\}$ in $\mathcal{H}_E$, we have that

$$(\phi, (\mathrm{tr}^E R)\psi)_S \overset{(***)}{=} \underbrace{\sum_i \langle \phi \otimes x_i, R(\psi \otimes x_i)\rangle}_{=: (\phi, \tilde{\rho}\psi)_S}$$

Pf: Let $\rho := \mathrm{tr}^E R$. Then, by definition,

$$(\phi, \rho\psi)_S = \mathrm{tr}_S(Q\rho), \text{ where } Qf := |\psi\rangle\langle\phi|f\rangle.$$

Then

$$(\phi, \rho\psi)_S = \mathrm{tr}_{SE}(QR)$$

$$= \sum_{i,j} (\phi_i \otimes \chi_j, Q(\phi_i \otimes \chi_j))$$

$\{\phi_i\}$ and $\{\chi_i\}$ are orthonormal bases for $\mathcal{H}_S$ & $\mathcal{H}_E$

$$= \sum_{i,j} \langle \phi_i \otimes \chi_j, (Q\phi_i) \otimes \chi_j \rangle$$

$$= \sum_i \langle \phi_i, \tilde{\rho} Q \phi_i \rangle$$

Def. of Q:
$Qf := |\psi\rangle\langle\phi|f\rangle$

$$= \sum_i \langle \phi_i, \tilde{\rho}\psi \rangle_S \langle \phi, \phi_i \rangle_S$$

$$= \Big\langle \sum_i \underbrace{\overline{\langle \phi, \phi_i \rangle}}_{= \langle \phi_i, \phi \rangle} \phi_i, \tilde{\rho}\psi \Big\rangle_S$$

$$= \Big(\underbrace{\sum_i \langle \phi_i, \phi \rangle \phi_i}_{= \phi \text{ since } \{\phi_i\} \text{ is an orthon. basis of } \mathcal{H}_S}, \tilde{\rho} \psi \Big)_S$$

$$\Rightarrow \quad (\phi, (\mathrm{tr}^E R) \psi)_S = \langle \phi, \tilde{\rho} \psi \rangle_S \quad \forall \phi, \psi \in \mathcal{H}_S$$

$$\Rightarrow \quad \mathrm{tr}^E R = \tilde{\rho}.$$

$\blacksquare$

<u>Prop</u>: There is a 1-1 correspondence between sesquilinear forms and operators

$$q(\phi, \psi) \longleftrightarrow B \text{ (bdd op.)}$$

From B, define $q(\phi, \psi) := \langle \phi, B\psi \rangle$

From $q(\phi, \psi)$, get Riesz to define the operator B uniquely from $q(\phi, \psi) = \langle \phi, B\psi \rangle$.

Claim: tr^E is positive. That is

tr^E (positive op.) = positive op.

Pf: Let $R \geq 0$, by (***), $\forall \phi \in \mathcal{H}_S$

$$\langle \phi, \mathrm{tr}^E R \phi \rangle_S = \sum_i \langle \underbrace{\phi \otimes x_i}_{\psi_i}, R(\underbrace{\phi \otimes x_i}_{\psi_i}) \rangle_{SE}$$

$$R \geq 0 \longrightarrow \geq 0 \Rightarrow \mathrm{tr}^E R \geq 0.$$

$\square$

Claim: $\mathrm{tr}^E(BR) = B\,\mathrm{tr}^E R \quad \forall B$ acting on $\mathcal{H}_S$.

Pf: We have that

$$\langle \phi, \mathrm{tr}^E(BR)\psi \rangle_S \overset{(***)}{=} \sum \langle \phi \otimes x_i, BR(\psi \otimes x_i) \rangle_{SE}$$

$$= \sum \langle B^*(\phi \otimes x_i), R(\psi \otimes x_i) \rangle_{SE}$$

$$= \sum \langle (B^*\phi) \otimes x_i, R(\psi \otimes x_i) \rangle$$

$$\overset{(***)}{=} \langle B^* \phi, (\mathrm{tr}^E R)\psi \rangle_S$$

$$= \langle \phi, B(\mathrm{tr}^E R)\psi \rangle_S$$

$$\forall \psi, \phi \in \mathcal{H}_S.$$

$\square$

Claim: tr^E is trace preserving; i.e.,

$$\mathrm{tr}^S \circ \mathrm{tr}^E = \mathrm{tr}$$

LECTURE 13 — REDUCED DYNAMICS

25/10/2023

Last lecture: For compound system $T = SE$, defined the PARTIAL TRACE $\mathrm{tr}^E : \{\text{density op. on } T\} \to \{\text{density op. on } S\}$.

Equivalent definitions: $\mathrm{tr}_S(A\, \mathrm{tr}^E R) = \mathrm{tr}_T(AR)$

coordinate free $\rightarrow$ $\forall$ S observable A

$$\Updownarrow$$

$$\langle \phi, (\mathrm{tr}^E \rho)\psi \rangle = \sum_j \langle \phi \otimes \eta_j, (\rho\psi) \otimes \eta_j \rangle$$

for some orthonormal basis $\{\eta_j\}$ of $\mathcal{H}_E$.

<u>HW</u>: Show that this is basis independent (Riesz).

$l : X \to \mathbb{R}$ is a linear bounded op. $\overset{\text{def.}}{\iff}$ $l \in X^*$

e.g., $X = L^p$, $p \in [1, \infty) \Rightarrow X^* = L^q$ w/ $\frac{1}{p} + \frac{1}{q} = 1$

$l : L^p \to \mathbb{C}$ lin. bdd functional $\overset{\simeq}{\longleftrightarrow} f \in L^q$

$L : \{\text{Bdd op.}\} \to \mathbb{C}$ $\overset{\simeq}{\longleftrightarrow}$ trace-class S_1 op. ρ

$\nwarrow S_\infty$ (Schatten)

$L(A) = \mathrm{tr}_T(A\rho)$ $\forall A$ bdd op. on $\mathcal{H}_S$

$(A \in S_\infty(\mathcal{H}_S))$

$\Rightarrow \exists \rho \in S_1(\mathcal{H}_S)$ s.t. $L(A) = tr_S(A\rho)$.

Consider the von Neumann equation

$R_{t=0} = R_0$

(vN) $$\partial_t R_t = -\frac{i}{\hbar}[H_T, R_t]$$

where H_T is the quantum Hamiltonian of the total space T.

Recall: $(vN) \Longleftrightarrow R_t = \alpha_t(R_0) := U_t^T R_0 U_t^{T\,*}$

where $U_t^T := e^{-iH_T t/\hbar}$ is the usual propagator for $i\hbar\,\partial_t \psi_t = H_T \psi_t$.

PROPERTIES OF α: (HW prove these)

(i) Linear

(ii) Positive (i.e., positive $\mapsto$ positive)

(iii) Trace preserving ($tr\, \alpha_t(\cdot) = tr(\cdot)$)

(iv) Commutes w/ taking adjoints

(v) Group homomorphism: $\alpha_t(AB) = \alpha_t(A)\alpha_t(B)$

(vi) $\alpha_s \circ \alpha_t = \alpha_{s+t} = \alpha_t \circ \alpha_s$.

(vii) $(\alpha_t)^{-1} = \alpha_{-t}$, $\alpha_0 = id$.

REDUCED DYNAMICS:

Density operator of the enviroment (positive)

$$\beta_t(\rho_0) := tr^E\left[\alpha_t(\rho_0 \otimes e_0)\right]$$

$\rho_t = \beta_t(e_0)$ reduced density op.

PROPERTIES:

- β_t depends on e_0
- β_t maps pure states onto mixed states

(pure states = rank 1 projections $\Longleftrightarrow$ wave fct. in QM
mixed states = not pure states; i.e., not rank 1 proj.)

Obs: α_t QM evolution maps pure states onto pure states.

PROPERTIES OF β_t: (HW prove these)

(i) Linear (b/c composition of linear operators.)

$\beta_t = tr^E \circ \alpha_t \circ$ (tensor w/ ϱ_0)
all linear

(ii) Positive (composition of positive ops.)

ϱ_0 is positive since density op.

(iii) Trace preserving

(iv) Commutes w/ adjoints (since composition of ops. that commute w/ adjoint)

(v) $\boxed{\beta_t \text{ is a 1-parameter group}} \iff \boxed{S \text{ and } E \text{ are } \underline{\text{not}} \text{ coupled}}$

$\Updownarrow$

$$\boxed{\alpha_t^T = \alpha_t^S \otimes \alpha_t^E} \iff \boxed{H_T = H_S \otimes Id_E + Id_S \otimes H_E}$$

(if there is a "$+W$", where W acts on $\mathcal{H}_S$ <u>and</u> $\mathcal{H}_E$ then we say S and E are coupled)

Thm: (Kraus) β_t is of the form

$$\beta_t(\rho) = \sum_j V_j \rho V_j^*$$

where V_j are bdd operators s.t. $\sum_j V_j V_j^* = \mathrm{Id}$.

Pf: (Idea) Use

$$\langle \phi, \beta_t(\rho)\psi \rangle = (\phi, \operatorname{tr}^E \alpha_t(\rho_0 \otimes e_0)\psi)$$

$$= \sum_j \left(\phi \otimes x_j, (\alpha_t(\rho_0 \otimes e_0)\psi) \otimes x_j\right)$$

where $\{x_j\}$ is an orthon. basis for $\mathcal{H}_E$. Choose x_j s.t. eigenfcts. of $e_0 \rightsquigarrow e_0 x_j = \lambda_j x_j$.

$$e_0 = \sum \lambda_k |x_k\rangle\langle x_k| \Rightarrow \text{result.}$$

$\square$

Lecture 14

27/10/2023

Reduced Dynamics

Reduced Dynamics: $\beta_t(\rho_0) \overset{(*)}{:=} \mathrm{tr}^E(\alpha_t(\rho_0 \otimes e_0))$

e_0 = density operator on E

α_t = total evolution $\alpha_t \equiv U_t^T (U_t^T)^*$, where $T = SE$

$U_t^T = e^{-iH_T t/\hbar}$ total Schrödinger evolution

We also have the following theorem:

Thm 1: β_t is

- Linear
- Positive
- Trace-preserving
- Commutes w/ adjoints

Thm 2: (Kraus) We can write

$$\beta_t(\rho) = \sum_n V_n \rho V_n^* \qquad (**)$$

where V_n are bounded and s.t. $\sum_n V_n V_n^* = Id$.

Thm 2 $\Rightarrow$ Thm 1 ✓

Thm 2 $\not\Leftarrow$ Thm 1 No!

$(**) \Rightarrow (*)$? Yes!

Obs: Thm 2 states $(*) \Rightarrow (**)$

NOTATION: !

- $S_1 = \left\{ \begin{matrix} \text{space of trace-} \\ \text{class operators} \end{matrix} \right\} = \left\{ \lambda : \underbrace{tr\sqrt{\lambda^*\lambda}}_{\|\lambda\|_{S_1}} < \infty \right\}$

Complete Banach

- $S_1^+ = \left\{ \begin{matrix} \text{space of den-} \\ \text{sity operators} \end{matrix} \right\} = \left\{ \lambda \in S_1 : \lambda \geq 0 \right\}$

- $M_k = \{ k \times k \text{ matrices} \}$

- $S_1 \otimes M_k = \{ [\rho_{ij}]_{k\times k} : \rho_{ij} \in S_1 \}$ ← matrix whose entries are S_1-operators

Def: (COMPLETELY POSITIVE) We say an operator $\beta_t \equiv \beta : S_1 \to S_1$ is completely positive iff the map $\beta \otimes Id_{M_k}$ on $S_1 \otimes M_k$ is positive $\forall\, k \geq 1$. Note that, in general

$$\beta \otimes Id \text{ maps } [\rho_{ij}] \xmapsto{\beta\otimes Id} [\beta(\rho_{ij})]$$

Say CPTP = completely positive trace-preserving.

Thm 3: $(**) \Leftrightarrow$ CPTP $\Rightarrow$ Thm 1 $\not\Rightarrow$ Thm 2.

Pf: $(\Rightarrow)$ let

$$\beta(\rho) = \sum_n V_n \rho V_n^*, \quad \sum_n V_n V_n^* = Id.$$

Then

$$(\beta \otimes Id)[\rho_{ij}] \overset{def}{=} [\beta(\rho_{ij})] = \left[\sum_n V_n \rho_{ij} V_n^* \right]$$

$$= \sum_n [V_n \rho_{ij} V_n^*]$$

$$= \sum_n (V_n \otimes Id)[\rho_{ij}](V_n \otimes Id)^*$$

Now, if we take

$$[\rho_{ij}] \geq 0 \Rightarrow (\beta \otimes Id)[\rho_{ij}] \geq 0$$

$R \geq 0 \Leftrightarrow \langle \psi, R\psi \rangle \geq 0$

Then $WRW^* \geq 0$ since

$\langle \psi, WRW^* \psi \rangle = \langle \phi, R\phi \rangle \geq 0$

($\Leftarrow$) Kraus Theorem.

$\blacksquare$

Upshot:

$\boxed{\beta_t \text{ is reduced dynamics}} \Longleftrightarrow \boxed{\beta_t \text{ is } \underbrace{\text{CPTP}}}$

Called QUANTUM DYNAMICAL MAPS
= QUANTUM COMMUNICATION CHANNELS

Q: $(**) \implies (*)$?

A: Yes by the above.

Def: The pair (S_1^+, β_t) is called a QUANTUM OPEN SYSTEM (generalizes quantum statistics)

//

DUAL DYNAMICS: The dual space to S_1 is:

$$S_1^* = \mathcal{A} := \{\text{bounded linear functionals on } S_1\}$$

Write $\omega(A) := tr(\rho A)$ for some S_1

$$\iff (\rho, A) : \begin{array}{ll} A \to \mathbb{R} & (\text{if } \rho \text{ fixed}) \\ S_1 \to \mathbb{R} & (\text{if } A \text{ fixed}) \end{array}$$

Given $\beta : S_1 \to S_1$, define $\beta^* : \mathcal{A} \to \mathcal{A}$ by

$$(\beta(\rho), A) = (\rho, \beta^*(A)) \quad \forall A \in \mathcal{A}.$$

<u>Obs</u>: $(S_\infty)^* = S_1$ ← unlike with Lebesgue spaces: $(L^\infty)^* \neq L^1$.

$\mathcal{A}^* \ni \omega$, $\omega(A) := \mathrm{tr}(A\rho)$ for some $\rho \in S_1$

then $|\omega(A)| \leq \|A\|_{S_\infty} \|\rho\|_{S_1}$.

$\Rightarrow$ tr bounded linear op, hence $\mathrm{tr} \in S_1^*$

<u>Digression</u>: X Banach $\rightsquigarrow$ $X^* = \{$bdd lin. functionals on $X\}$

$= \{ \ell : \ell : X \to \mathbb{C} \text{ linear, bdd} \}$

Then X^* is again a Banach space w/ norm

$$\| \ell(\rho) \|_{X^*} = \sup_{\rho \neq 0} \frac{|\ell(\rho)|}{\|\rho\|_X} \quad \text{in } X^*$$

If $\beta : X \to X$, then define $\beta^* : X^* \to X^*$ as

$$(\beta^* \ell)(\rho) = \ell(\beta(\rho)).$$

We can write this $\ell(\rho) = (\rho, A)$ for some $A \in X^*$.

Consider $\beta : S_1 \to S_1$. Note that this means that we can define $\beta^* : S_1^* := \mathcal{A} \to \mathcal{A}$ as

$$(\beta(\rho), A) = (\rho, \beta^*(A)).$$

Duality determines it uniquely

Then,

$$\beta \text{ trace preserving}$$
$$\Updownarrow$$
$$\mathrm{tr}(\beta(\rho)) = \mathrm{tr}(\rho)$$
$$\Updownarrow$$
$$\beta^* \text{ is } \underline{\text{UNITAL}}$$
$$\Updownarrow$$
$$\beta^*(\mathrm{Id}) = \mathrm{Id}$$

LECTURE 14

01/11/2023

DUAL DYNAMICS

Recall: <u>States</u> $\longleftrightarrow$ density operators $\rho \in S_1^+ \subset S_1$

Schatten space of trace-class operators.

<u>Observables</u> $\longleftrightarrow$ $A \in \mathcal{A} := \{\text{bdd operators}\}$

Coupling: $(\rho, A) \overset{(\#)}{=} \operatorname{tr}(\rho A)$ $\left(\begin{array}{c} A \text{ bdd}, \ \rho \in S_1^+ \\ \Downarrow \\ A\rho, \ \rho A \in S_1 \end{array} \right)$

Average of A in state ρ

Hölder inequality: $|\operatorname{tr}(A\rho)| \leq \|\rho\|_{S_1} \|A\|$

Map β of S_1 $\xrightarrow{\text{dualize}}$ map β^* (dual) of $\mathcal{A}$

$$(\#\#) \quad (\rho, \beta^*(A)) = (\beta(\rho), A), \quad \begin{array}{l} \forall \rho \in S_1^+ \\ \forall A \in \mathcal{A} \end{array}$$

Claim: Quantum map β is CPTP

$\Downarrow$

β^* is completely positive and unital

That is: (a) β^* is completely positive

(b) β^* is unital (i.e., $\beta^*(\mathrm{Id}) = \mathrm{Id}$)

(c) β^* is a $*$-map; i.e., commutes w/ taking adjoints (i.e., $\beta^*(A^*) = (\beta^*(A))^*$)

NOTE: β CP $\Rightarrow$ β^* CP

$$\beta \text{ CP} \Leftrightarrow \beta(\rho) = \sum_{n\in I} V_n \rho V_n^* \quad \left(\begin{matrix}\text{bdd ops.}\\ V_n\end{matrix}\right)$$

countable set

$$\Downarrow \; {\color{red}(\#\#)}$$

$$\beta^*(A) = \sum_{n\in I} V_n^* A V_n$$

$$\mathrm{tr}(V\rho V^* A) \overset{\text{cyclicity}}{=} \mathrm{tr}(\rho V^* A V)$$

β TP $\Rightarrow$ β^* unital

$$\mathrm{tr}\,\rho = \mathrm{tr}(\beta(\rho)) = \mathrm{tr}(\beta(\rho)\,\mathrm{Id}) \overset{(\#)}{=} (\beta(\rho), \mathrm{Id})$$

$$\mathrm{tr}\,\rho = \mathrm{tr}(\rho\,\mathrm{Id}) \overset{(\#)}{=} (\rho, \mathrm{Id})$$

$$(\beta(\rho), \mathrm{Id}) \overset{(\#\#)}{=} (\rho, \beta^*(\mathrm{Id}))$$

$$\Rightarrow (\rho, \mathrm{Id}) = (\rho, \beta^*(\mathrm{Id})) \quad \forall \rho \in S$$

$$\Rightarrow \beta^* \text{ unital}$$

Thm: (DUAL STINESPRING)

β^* (dual map) is completely positive unital $\iff$ $\exists$ Hilbert space $\mathcal{K}$ and $W : \mathcal{H} \to \mathcal{H} \otimes \mathcal{K}$ s.t.

$$\beta^*(A) = W^*(A \otimes \mathrm{Id}_{\mathcal{K}})W$$

(such $\mathcal{K}$ is called ANCILLA SPACE)

NOTE: $\langle W^* f, g \rangle_{\mathcal{H}} = \langle f, Wg \rangle_{\mathcal{H}\otimes\mathcal{K}}$.

Pf: $(\Rightarrow)$ Let β be CP $\Rightarrow \beta^*(A) = \sum_{i\in I} V_i^* A V_i$,

V_i bdd & $\sum_{i\in I} V_i^* V_i < \infty$.

$$\mathcal{K} := \ell^2(I) = \{ (x_i)_{i\in I} : \sum |x_i|^2 < \infty \}$$

Then $\mathcal{H} \otimes \mathcal{K} \overset{HW}{=} \underbrace{\mathcal{H} \times \cdots \times \mathcal{H}}_{|I| \text{ times}} = \{ \vec{\psi} = \underbrace{\psi \oplus \cdots \oplus \psi}_{|I| \text{ times}} \} = \{ (\psi_i)_{i\in I} : \psi_i \in \mathcal{H} \}$

with the inner product $\langle \vec{\psi}, \vec{\phi} \rangle_{\mathcal{H}\times\cdots\times\mathcal{H}} = \sum_{i\in I} \langle \psi_i, \phi_i \rangle_{\mathcal{H}}$

Define the map W by

$$\mathcal{H} \ni \psi \xmapsto{W} \bigoplus_{i\in I} V_i^* \psi \in \bigoplus \mathcal{H}$$

Then we get the dual map

$$\bigoplus \mathcal{H} \ni \bigoplus_{i\in I} \psi_i \xmapsto{W^*} \sum_{i\in I} V_i \psi_i \in \mathcal{H} .$$

Compute $W^*(A \otimes \mathrm{Id}_{\mathcal{K}}) W \psi$:

$$W^*(A \otimes \mathrm{Id}_{\mathcal{K}}) W \psi \overset{\text{def}}{=} W^*(A \otimes \mathrm{Id}_{\mathcal{K}}) \bigoplus_{i\in I} V_i^* \psi$$

$$= W^* \bigoplus_{i\in I} A V_i^* \psi$$

$$\overset{\text{def}}{=} \sum_{i\in I} V_i A V_i^* \psi$$

$$= \beta^*(A) \psi .$$

($\Leftarrow$) Tautology from def.

$\square$

Lecture 15

03/11/2023

Entalglement

Def: (Entalgled Systems) Subsystems A and B are entalgled in $\Psi_{AB} \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$ iff it can't be decomposed into each space

i.e., $\forall \phi_A \in \mathcal{H}_A$, $\forall \psi_B \in \mathcal{H}_B$, $\Psi_{AB} \neq \phi_A \otimes \psi_B$.

very hard to determine if states in $\mathcal{H}_{AB}$ are indeed entangled...

Thm: (Entanglement Criterion) ECT

Ψ_{AB} entangled $\iff$ Reduced density operator $\rho_A := \mathrm{tr}_B(P_{\Psi_{AB}})$ has rank > 1

rank := dim im ρ_A

Pf: Derive this entalglement criterion (ETC) from Spectral Decomposition Theory (SDT):

Thm: (Schmidt Decomposition) $\forall\, \Psi_{AB} \in \mathcal{H}_{AB}$, there exists $p_j \geq 0$ satisfying $\sum_j p_j = \|\Psi_{AB}\|^2_{AB}$ and there exists orthonormal bases $\{\phi_j^A\}$ of $\mathcal{H}_A$ and $\{\psi_j^B\}$ of $\mathcal{H}_B$ s.t.

$$\Psi_{AB} = \sum_k \sqrt{p_k}\, \overbrace{\phi_k^A \otimes \psi_k^B}^{\text{NOT a basis in } \mathcal{H}_{AB}!}\,.$$

Prop: $$\rho_A = \sum_j p_j\, |\phi_j^A\rangle\langle\phi_j^A|\,.$$

Pf: $$\rho_A \overset{\text{def}}{=} \operatorname{tr}_B(P_{\Psi_{AB}}) \overset{\text{def}}{=} \sum_j \langle \psi_j^B, P_{\Psi_{AB}}\, \psi_j^B \rangle$$

$P_{\Psi_{AB}} \overset{\text{def}}{=} |\Psi_{AB}\rangle\langle\Psi_{AB}|$

$\langle\cdot|\cdot\rangle_B$ is inn. prod. in $\mathcal{H}_B$ only.

$$= \sum_j \langle \underset{\in\, \mathcal{H}_B}{\psi_j^B} | \underset{\in\, \mathcal{H}_{AB}}{\Psi_{AB}} \rangle_B \langle \Psi_{AB} | \psi_j^B \rangle_B$$

Schmidt Dec.:

$$\langle \Psi_{AB} | \psi_j^B \rangle_B = \sqrt{p_j}\, \langle \phi_j^A |$$

$$\langle \psi_j^B | \Psi_{AB} \rangle_B = \sqrt{p_j}\, | \phi_j^A \rangle$$

$$= \sum_j p_j\, |\phi_j^A\rangle\langle\phi_j^A| .$$

$\square$

Upshot: When applying ρ_A to fcts on $\mathcal{H}_A$:

"Actual" full inn. product

$$\langle g, \rho_A f \rangle_A = \sum_j \langle g \otimes \psi_j^B | \Psi_{AB} \rangle_{AB} \langle \Psi_{AB} | f \otimes \psi_j^B \rangle_{AB}$$

Schmidt Decomp.

$$= \sum_k \sqrt{p_k}\, \langle g \otimes \psi_j^B | \phi_k^A \otimes \psi_k^B \rangle$$

$$= \sum_k \sqrt{p_k}\, \langle g, \phi_k^A \rangle \underbrace{\langle \psi_j^B, \psi_k^B \rangle}_{= \delta_{jk}}$$

$$= \sqrt{p_j}\, \langle g | \phi_j^A \rangle .$$

HW: Ψ_{AB} not entangled iff, in the Schmidt decomposition, we have

$$P_k = \begin{cases} 1, & k = k_0 \\ 0, & k \neq k_0 \end{cases} \qquad \left(\text{i.e., } \Psi_{AB} = \phi_{k_0}^{A} \otimes \psi_{k_0}^{B} \right)$$

($\Leftarrow$) Obvious

($\Rightarrow$) $\Psi_{AB} = x \otimes y$ for some $x \in \mathcal{H}_A$, $y \in \mathcal{H}_B$

WTS: $P_k = \delta_{k,k_0}$.

• Derive Schmidt Decomposition from Schmidt Dec. for operators:

SDCO

Thm: (Schmidt Decomposition for Operators) For any Hilbert-Schmidt ~~compact~~ operator $K : \mathcal{H}_B \to \mathcal{H}_A$ $\exists \{\lambda_j\}$, $\lambda_j \geq 0$ $\forall j$, $\sum_j \lambda_j^2 < \infty$, $\cancel{\lambda_j \to 0}$ and bases $\{\phi_k^A\}$ of $\mathcal{H}_A$ and $\{\psi_j^B\}$ of $\mathcal{H}_B$ s.t.

Much stronger than compact.

$$K = \sum_k \lambda_k \, |\phi_k^A\rangle\langle\psi_k^B| \, .$$

Def: $T \in \mathcal{L}(X,Y)$ is compact iff the image of the unit ball of X is precompact in Y.

Ex: Finite rank ops. are compact.

Claim: SDTO $\Rightarrow$ SDT

Pf: Pick bases $\{e_j^A\}$ and $\{f_j^B\}$. then get a basis $\{e_j^A \otimes f_j^B\}$ for $\mathcal{H}_{AB}$. Then

$$\psi_{AB} = \sum_{ij} c_{ij}\, e_i^A \otimes f_j^B, \quad \sum_{ij} |c_{ij}|^2 = \|\psi_{AB}\|^2$$

$$\mathcal{H}_{AB} \ni \psi_{AB} \overset{1-1}{\longleftrightarrow} \boxed{\text{Hilbert Schmidt}} \text{ operator } K : \mathcal{H}_B \to \mathcal{H}_A$$

$$\psi_{AB} \overset{1-1}{\longleftrightarrow} K = \sum_{ij} c_{ij}\, |e_i^A\rangle\langle f_j^B|$$

$\leftarrow$ NTS: indep. of basis

K is Hilbert-Schmidt $\Leftrightarrow$ $\mathrm{tr}(K^* K) < \infty$

$\{$Hilbert-Schmidt ops.$\}$ is a Hilbert space w.r.t. $\langle K, M\rangle = \mathrm{tr}(K^* M)$

Schatten space S_2.

For $K = \sum c_{ij} |e_i^A\rangle\langle f_j^B|$, use SCTO to get $\{\lambda_k\}$, $\lambda_k \geq 0$ & $\sum \lambda_k^2 < \infty$ ~~$\lambda_k(\ldots)$~~, and bases $\{\phi_j^A\}$ of $\mathcal{H}_A$ and $\{\psi_j^B\}$ of $\mathcal{H}_B$ s.t.

Hilbert-Schmidt $\Rightarrow \sum_k \lambda_k^2 < \infty$

$$K = \sum_k \lambda_k |\phi_k^A\rangle\langle\psi_k^B|$$

$$\Longrightarrow \Psi_{AB} = \sum_k \lambda_k \, \phi_k^A \otimes \psi_k^B,$$

with

$$\|\Psi_{AB}\|^2 = \sum_k \lambda_k^2 < \infty$$

Define $p_k := \sqrt{\lambda_k}$.

$\square$

Upshot:

$$\boxed{\Psi_{AB} \text{ is entangled}} \iff \boxed{\rho_A := \mathrm{tr}_B(P_{\Psi_{AB}}) \text{ has rank } (= \dim \operatorname{im} \rho_A) > 1}$$

Computationally detect this entanglement:

$$E(\Psi_{AB}) = \underbrace{S}(\rho_A)$$

$S(\rho) := -\operatorname{tr}(\rho \log \rho)$ "von Neumann Entropy of ρ"

density operator

* **VON NEUMANN ENTROPY**: S acts on density operators ρ (i.e, $\rho \geq 0$ and $\operatorname{tr}\rho = 1$).

HW: $\|\rho\| \leq \operatorname{tr}\rho = 1$ (this is true b/c $\|\rho\| = \max\{\text{eigenvals.}\} \leq \sum\{\text{eigenvals}\}$)

$\Updownarrow$

Now, $0 \leq \rho \leq 1$. Define $f(\lambda) = -\lambda \log \lambda$, for $0 \leq \lambda \leq 1$. Then

$$\lambda \log \lambda = \lambda \sum_{n=0}^{\infty} \frac{1}{n}(1-\lambda)^n.$$

So,

$$\boxed{f(\rho) := \rho \sum_{n=0}^{\infty} \frac{1}{n}(1-\rho)^n.}$$

Cauchy - Formula: $f(\lambda) = \frac{1}{2\pi i}\int_\gamma \frac{f(z)}{\lambda - z}\, dz$

$\Rightarrow f(A) = \frac{1}{2\pi i}\oint_\gamma \frac{f(A)}{A-z}\, dz$

A away from zero.

Claim: $f(\rho)$ is

- bounded
- self-adjoint
- Eigenvals. of $f(\rho) = \{ f(\lambda_j) : \lambda_j$ eigenvals. of $\rho \}$

  exist, isolated, b/c ρ compact and between 0 and 1

- $\| f(\rho) \| \leq \sup_{\lambda \in [0,1]} | f(\lambda) |$

- $f(\rho)$ is trace-class $\Leftrightarrow \sum_j |f(\lambda_j)| < \infty$

Then, we can define $S(\rho) = - \operatorname{tr} f(\rho)$.

Claim: $S(\rho) = 0 \Leftrightarrow \rho$ is a rank 1 projection.

Pf: $S(\rho) = - \sum \lambda_j \log \lambda_j = 0 \Leftrightarrow \lambda_j = \delta_{j,j_0}$

(mult. $\lambda_{j_0} = 1$ since $\operatorname{tr} \rho = 1$).

LECTURE 16

EVOLUTION OF QM & QI

15/11/2023

If system $\mathcal{H}_{SE} = \mathcal{H}_S \otimes \mathcal{H}_E$ is described by wave-fct. $\Psi \in \mathcal{H}_{SE}$ then

$\exists \phi \in \mathcal{H}_S$ s.t. $\langle \Psi, (A \otimes Id_E)\Psi \rangle_{SE} = \langle \phi, A\phi \rangle_S \;\; \forall A$ acting on S.

$\iff \Psi = \phi \otimes \eta$ for some $\eta \in \mathcal{H}_E$

$\iff \mathcal{H}_S$ and $\mathcal{H}_E$ are not correlated.

GOAL: Extend the notion of state so that for all state ω_{SE} of $\mathcal{H}_{SE}$, there exists a state ω_S of S s.t. $\forall A$ acting on S, $\omega_S(A) = \omega_{SE}(A \otimes Id_E)$.

This would allow integrating out any unknown information.

* DENSITY OPERATORS: Generalize orthogonal proj. to general positive trace-class ops. Γ on $\mathcal{H}$ called density operators s.t. $tr(A P_\Psi) \rightsquigarrow tr(A\Gamma)$.

Observables $A \iff$ Random variables X

Density operators $\Gamma \iff$ Probability dist. dP

Quantum average $\mathrm{tr}(A\Gamma) \Longleftrightarrow$ Classical average $\int X \, dP$.

REDUCED DENSITY OPERATORS:

Thm: $\forall$ total density operator Γ, $\exists!$ system density op. γ s.t. $\forall$ system obs. A,

$$\underbrace{\mathrm{tr}_{SE}}\big((A \otimes \mathrm{Id}_E)\Gamma\big) = \underbrace{\mathrm{tr}_S}(A\gamma)$$

standard traces on these spaces.

coörd. free definition

Denote by tr_E the <u>unique</u> map $\mathrm{tr}_E : \Gamma \mapsto \gamma$.

partial trace

$\gamma = \mathrm{tr}_E \Gamma$ is a density op. on S ("reduced DO").

If ψ satisfies (SE), then the density op. $\Gamma = P_\psi$ satisfies von Neumann's eq.

QUANTUM STATISTICS:

Mixed states:

$$\Gamma = p_1 P_{\psi_1} + p_2 P_{\psi_2}$$

- States: DOs
- Evolution: von Neumann eq.
- Observables: self-adjoint ops. A
- Averages: $\langle A \rangle_\Gamma := \mathrm{tr}(A\Gamma)$

REDUCED DYNAMICS: Evolution is

$$\partial_t \Gamma_t = -\frac{i}{\hbar}[H, \Gamma_t], \quad \Gamma|_{t=0} =: \gamma_0 \otimes \rho_E .$$

Thus, the reduced DO of S at time t is

$$\beta_t(\gamma_0) := \mathrm{tr}_E \, \Gamma_t .$$

- β_t is irreversible (dissipative)
- β_t : pure states $\longmapsto$ mixed states
- S and E <u>not</u> interacting $\Rightarrow$ β_t unitary evolution of S

$$\beta_t = \alpha_t^S ,$$

where

$$\alpha_t^S(\gamma) = e^{-iH_S t/\hbar} \gamma_0 \, e^{iH_S t/\hbar}$$

LECTURE 17

22/11/2023

GENERAL CONSTRAINTS ON PROPAGATION OF QUATUM INFO.

LOCALIZATION: We have 3 objects: observables, states, and Q maps.

Consider $X \subset \mathbb{R}^m$ (or a lattice $\mathbb{Z}^m$).

Obs. A is localized in X $\Longleftrightarrow$ $A \chi_{X^c} = \chi_{X^c} A = 0$.

State ρ is localized in X $\iff$ $\mathrm{tr}(\chi_{X^c}\rho) = 0$

Quantum map β is localized in X $\iff$ β maps states in X to states in X.

RESTRICTION: of A to X = $A_X := \chi_X A \chi_X$

of ρ to X = $\rho_X := \chi_X \rho \chi_X$

$$\left[\ \mathrm{tr}(\chi_{X^c}\rho_X) = 0 \quad \text{and} \quad \mathrm{tr}(A_X\rho) = \mathrm{tr}(A\rho_X) = \mathrm{tr}(A_X\rho_X)\ \right]$$

* **CONTROL OF QUANTUM STATES:** The goal is to manipulate states in X to create a "desired state" in a set Y.

Let τ be a quantum map localized in X.

"Control map"

assume ρ is also localized in X

(i) Apply τ to states: $\rho \overset{\tau}{\longmapsto} \tau(\rho) =: \rho^\tau$.

(ii) Evolve ρ^τ according to von Neumann evolution α_t (or equiv., β_t) to map $\rho^\tau \overset{\alpha_t}{\longmapsto} \alpha_t(\rho^\tau) =: \rho_t^\tau$.

(iii) Restrict this to Y by $\rho_t^\tau \longmapsto [\rho_t^\tau]_Y$.

Goal: make $[\rho_t^\varepsilon]_Y$ "close" to a given state σ.

CRITERION OF CLOSENESS: "Figure on merit (FOM)" determined by the fidelity

$$F([\rho_t^\varepsilon]_Y, \sigma)$$

if $F \approx 0$, we failed
if $F \approx 1$, we won ☺

We define the

FIDELITY: $F(\rho,\sigma) := \| \sqrt{\rho}\sqrt{\sigma} \|_1$

Obs: if ρ, σ are pure states (i.e., they are rank 1-projections) we have $\rho = \sqrt{\rho}$ and $\sigma = \sqrt{\sigma}$ $\rightsquigarrow$ $\rho = P_\phi$, $\sigma = P_\psi$. So,

$$\rho\sigma = |\phi\rangle\langle\phi|\psi\rangle\langle\psi| \rightsquigarrow |\rho\sigma|^2 = |\langle\phi,\psi\rangle|^2$$

$$\Rightarrow \| \sqrt{\rho}\sqrt{\sigma} \|_1 = tr(|\sqrt{\rho}\sqrt{\sigma}|) = |\langle\phi,\psi\rangle| .$$

Obs: $0 \leq F \leq 1$

clearly, b/c it is a norm

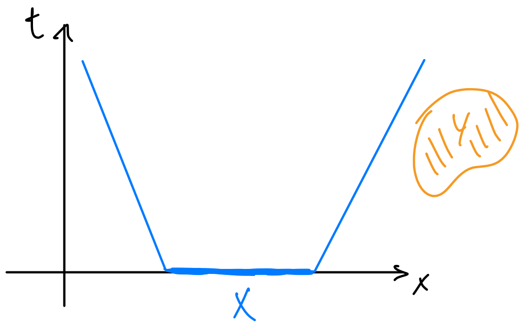
true by (non-abelian) Cauchy-Schwarz

We can also define another figure of merit using this fidelity F is:

$$F([\rho_t^\varepsilon]_Y, [\rho_t]_Y)$$ without the control

Then, if $F \simeq 1 \rightsquigarrow$ ineffective.

LIGHT-CONE ESTIMATION: Information cannot possibly reach Y in the case in the left.



Information travels at the effective speed of light.

Claim: $\exists c > 0$ s.t.

$$F\left([\rho_t^c]_Y, [\rho_t]_Y\right) \geq 1 - c\, d_{XY}^{-n},$$

for $t \leq \frac{1}{c} d_{XY}^{-n}$.

max. speed of propagation of info.

d_{XY} is distance (e.g., Euclidean)

$\Rightarrow$ Speed of propagation of information is not infinite!

* **QUANTUM MESSAGING**: Alice is in X and wants to send a message to Bob who is in Y. That is, Alice in X has obs. A (or, more generally, a quantum map τ). Bob has an obs. B in Y. Both have access to a state ρ.

PROTOCOL: Alice applies $\tau_r(\rho) := e^{-iAr} \rho\, e^{iAr} =: \rho^r$ and then applies α_t to ρ^r to get $\alpha_t(\rho^r) =: \rho_t^r$.

Bob perceives ρ_t^r and computes

$$\left| \operatorname{tr}(B\rho_t^r) - \underbrace{\operatorname{tr}(B\rho_t)}_{} \right| .$$

result Bob would get if there was no information in the message.

Claim: $\left|\operatorname{tr}(B\rho_t^r) - \operatorname{tr}(B\rho_t)\right| \leq \int_0^r \left| \operatorname{tr}([\underset{\text{loc. in } X}{A}, \alpha_t(\underset{\text{loc. in } Y}{B})]\rho^s)\right| ds$

LECTURE 18

24/11/2023

LIGHT CONE BOUNDS

LIGHT CONE BOUNDS: Dynamics from von Neumann

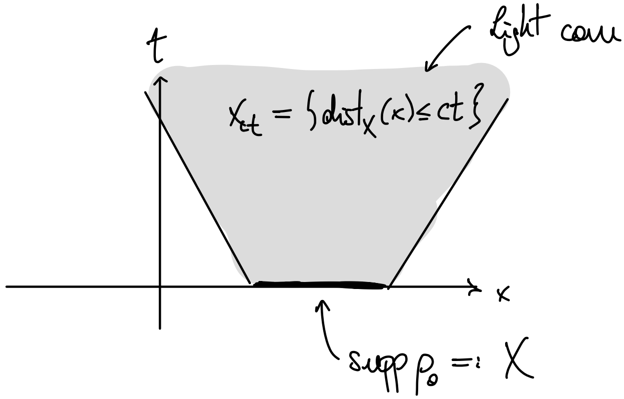
$$\partial_t \rho_t = -i\,[H, \rho_t] \quad \text{and} \quad \rho_t\big|_{t=0} =: \rho_0$$

$\hbar = 1$

where H = self-adjoint operator ($\hbar = 1$), $H = \omega(p) + V(x)$, $p = -i\nabla$

ρ = density operator on $\mathcal{H} = L^2(\mathbb{R}^n)$,

GOAL: Show that ρ_t is localized in the light cone given by supp ρ_0



$$\boxed{\mathrm{Prob}_{\rho_t}(x \notin X_{ct}) = \mathrm{tr}(\chi_{X_{ct}^c}\,\rho_t) \lesssim \frac{1}{t^n} \quad (*)}$$

- inf s.t. $(*)$ holds gives the max. speed of propagation.

Assumption:

(A) $\mathrm{ad}^k_{d_X}(H)$ is bounded for $k = 1, \dots, n$,

$d_X : x \mapsto d_X(x)$ and $\begin{cases} \mathrm{ad}^k_A(H) = [\mathrm{ad}^{k-1}_A(H), A] \\ \mathrm{ad}^0_A(H) = H \end{cases}$ (defined recursively)

Obs: If $H = -\Delta + V$, then (A) is not satisfied b/c

$[-\Delta, x] \overset{(A)}{=} -\nabla \longleftarrow$ not bounded!

On the other hand, the semi-relativistic Hamiltonian

$$H = \sqrt{-\Delta + m^2} + V \text{ satisfies (A)}$$

b/c

$$[H, x] = -\nabla_k \sqrt{|k|^2 + m^2}\,\Big|_{k=-i\nabla}$$

$$[\omega(p), x] = \nabla_k\, \omega(p)\,\Big|_{k=p}$$

Remark: If (A) is not satisfied, then (*) is not true

Thm: Assume (A) and that ρ_0 is localized in X.
Then $\exists k > 0$ such that

$$\mathrm{Prob}_{\rho_t}(x \notin X_{ct}) = \mathrm{tr}(\chi_{X_{ct}^c}\, \rho_t) \lesssim \frac{1}{t^n} \qquad (*)$$

$\forall c \geq k$ (max. speed) w/ n same as in (A)

Def: (PROPAGATION OBSERVABLES) Want to estimate

$$\omega_\rho(\phi_t) := \mathrm{tr}(\phi_t\, \rho_t) =: \langle \phi_t \rangle_{\rho_t},$$

where ϕ_t is a family of observables (i.e., bdd & self-adjoint ops.)

Define the <u>HEISENBERG DERIVATIVE</u> as:

$$\boxed{D\phi_t := \partial_t \phi_t + i[H, \phi_t]}$$

Obs: $\boxed{\partial_t \langle \phi_t \rangle_{\rho_t} = \langle D\phi_t \rangle_{\rho_t}.}$

Also, note that

$$\langle \phi_t \rangle_{\rho_t} = \langle \phi_0 \rangle_{\rho_0} + \int_0^t \langle D\phi_s \rangle_{\rho_s} \, ds$$

Want: $D\phi_t \le 0$ b/c then the average monotonically decreases (D is an "entropy").

Want: ϕ_t monotonically decreasing along evolution (just like entropy).

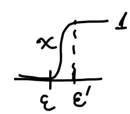
global thing

Next best thing: ϕ_t decreases along evolution to small and recursive terms.

recursive monotonicity

Define the PROPAGATION (IDENTIFIER) OBSERVABLE (PIO):

$$\chi_{ts} := \chi\left(\frac{1}{s}(d_X - ct)\right), \text{ where } \chi \text{ is } \left[\begin{array}{l} \text{smooth fct.} \\ \chi(r) = \begin{cases} 1, & r \ge \varepsilon' \\ 0, & r \le \varepsilon \end{cases} \end{array}\right.$$



Denote the space of such χ's as $\mathcal{F} := \{\chi\}$.

Prop: (Recursive Monotonicity Bound) $\forall \chi \in \mathcal{F}, \exists \tilde{\chi} \in \mathcal{F}$ s.t.

$\kappa := \|[H, d_X]\| \sim$ quantum speed, $\delta = c - \kappa > 0$

$$D\chi_{ts} \le -\frac{\delta}{s}\chi'_{ts} + \underbrace{\frac{c}{s^2}\tilde{\chi}'_{ts}}_{\text{recursive term}} + \underbrace{O(s^{-n})}_{\text{small}} \qquad \text{(RMB)}$$

$\chi'_{ts} := \chi'\left(\frac{1}{s}(d_X - ct)\right)$, $\chi'(\lambda) = \partial_\lambda \chi(\lambda)$.

$K := \| [H, d_X] \| \sim$ quantum speed. Velocity observable is $v = \dot{x}$
$\uparrow d_X \approx x$ for large x $\qquad = i[H,x]$
$K := \|v\| = \|[H,x]\|$

Proving the prop. above is hard (so we postpone it).

Pf: (of the theorem, assuming the proposition above)

Applying $\omega_t(\cdot) = \langle \cdot \rangle_t$ (i.e., taking the average and then integrating), we get: $t \le s$,

(IRMB)

$$\langle \chi_{ts} \rangle_t \le -\frac{\delta}{s} \int_0^t \langle \chi'_{rs} \rangle_r \, dr + \frac{C}{s^2} \int_0^t \langle \tilde{\chi}'_{rs} \rangle \, dr + O(s^{-n+1})$$

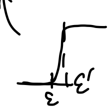
Take the average of (RMB) & use $\langle D\chi_{ts} \rangle_t = \partial_t \langle \chi_{ts} \rangle_t$.

and $\langle \chi_{ts} \rangle_t = \langle \chi_{0s} \rangle_0 + \int_0^t \langle D\chi_{rs} \rangle_r \, dr$

$$\Longrightarrow \langle \chi_{ts} \rangle_t \overset{(1)}{\le} \langle \chi_{0s} \rangle_0 - \frac{\delta}{s} \int_0^t \langle \chi'_{rs} \rangle_r \, dr$$
$$+ \frac{C}{s^2} \int_0^t \langle \tilde{\chi}'_{rs} \rangle_r \, dr + O(s^{-n+1}).$$

Claim: $\langle \chi_{0s} \rangle_0 = 0$

Indeed $\chi_{0s} \overset{\text{def}}{=} \underline{\chi}\left(\frac{1}{s} d_X\right) \neq 0$ only if $\frac{1}{s} d_X(x) \ge \varepsilon$



$\Longleftrightarrow d_X(x) = d(x, X) \ge \varepsilon s$

since ρ_0 localized at $X \Rightarrow \operatorname{tr}\left(x\left(\frac{1}{s}dx\right)\rho_0\right) = 0$.

Now, (IRMB) $\Rightarrow \langle x_{ts}\rangle_t \leq \frac{C}{s^2}\int_0^t \langle \underline{\tilde{x}'_{rs}}\rangle_r \, dr + O(s^{-n+1})$

$\tilde{x}'_{rs} \leq \sup|x'_{rs}| = \text{const.} = C/_{\varepsilon-\varepsilon'}$

$$\leq \frac{C_*}{s^2}\, t \leq \frac{C_*}{s}.$$

$\Rightarrow \langle x'_{rs}\rangle_r \overset{\text{def}}{=} \operatorname{tr}(x'_{rs}\rho_r)$

$= \operatorname{tr}\left(x'_{rs}\sqrt{\rho_r}\sqrt{\rho_r}\right)$

$\overset{\text{cyclicity}}{=} \operatorname{tr}\left(\sqrt{\rho_r}\,x'_{rs}\sqrt{\rho_r}\right)$

$\leq \|x'_{rs}\| \operatorname{tr}\left(\sqrt{\rho_r}\sqrt{\rho_r}\right)$

Average $\leq$ largest output

$= \underbrace{\sup|x'_{rs}| \operatorname{tr}(\rho_r)}_{=\text{const.}} < \infty$.

(IRMB) $\Rightarrow$

$$\boxed{\int_0^t \langle x'_{rs}\rangle_r \, dr \leq \frac{C}{s}\int_0^t \langle \tilde{x}'_{rs}\rangle_r \, dr + O(s^{-n+1}). \quad \text{(RB)}}$$

&, from above, $\boxed{\langle x_{ts}\rangle_t \leq \frac{C}{s} \quad \text{(AB)}}$ $\forall x \in \mathcal{F}, \exists \tilde{x} \in \mathcal{F}$ s.t.

So, apply (AB) to (RB):

(AB) here to find the bound

$$\boxed{\int_0^t \langle x'_{rs}\rangle_r \, dr \leq \frac{C}{s}\int_0^t \frac{C_*}{r}\, dr = \frac{C}{s} \quad \text{(AB2)}}$$

Now, apply (AB2) to (RB):

$$\int_0^t \langle x'_{rs}\rangle_r \, dr \leq \frac{C}{s}\cdot\frac{C}{s} = \frac{C}{s^2}.$$

Keep applying these estimatives...

$$\int_0^t \langle \tilde{x}'_{rs}\rangle_r \, dr \xrightarrow{\text{estimates}\ldots} \int_0^t \langle x'_{rs}\rangle_r \, dr$$

$$\int_0^t \langle \tilde{x}'_{rs}\rangle_r \, dr = O\left(\frac{1}{s^k}\right) \qquad \int_0^t \langle x'_{rs}\rangle_r \, dr = O\left(\frac{1}{s^{k+1}}\right) \quad \vdots$$

Iterate this until $k=n$. Then, we get

$$\boxed{\int_0^t \langle x'_{rs}\rangle_r \, dr \leq \frac{c}{s^n} \quad (ABn)}$$

Plug (ABn) into (IRBM) to get $\langle x_{st}\rangle_t \leq \frac{c}{s^n}$. ■

LECTURE 19

29/11/2023

APPLICATIONS OF LIGHT CONE BOUNDS

* Control of Quantum States: Control $\tau(\rho) = V\rho V^*$ w/ $V = e^A$, $\operatorname{supp} A \subset X$.

Here and beyond, consider only pure states

> **Prop 1:** $\forall \varepsilon > 0 \ \exists d_{XY}$ s.t. $F([\rho_t^V]_Y, [\rho_t]_Y) \geq 1-\varepsilon$ $\forall t \leq \frac{d_{XY}}{c}$.
>
> $\rho^V = V^* \rho V \to \rho_t^V := \alpha_t(\rho^V)$

Cor 1: It takes at least $\frac{d_{XY}}{c}$ time to control the state at

y from the set X.

* **Quantum Messaging:**

> **Prop 2**: supp $V \subset X$ and supp $B \subset Y$, then $\exists c > 0$ s.t.
>
> $$M := \left| tr(B\rho_t^V) - tr(B\rho_t) \right| \lesssim \frac{d_{XY}^{-n}}{c}$$
>
> $\forall t \leq \frac{d_{XY}}{c}$.

Cor 2: Bob would not see any message for $t \leq \frac{d_{XY}}{c}$

STUDY THIS FOR TEST

Pf: (Prop. 2) Use Light Cone Bound (LCB). Then

$tr(\chi_Y \rho_t) \leq c\, d_{XY}^{-n}$ for $t \leq \frac{d_{XY}}{c}$ outside of LC

Suppose $\rho = P_\phi$ (rank-1 proj.) $\rightsquigarrow P_{V\phi} = V \rho V^*$

not normalized

Recall: $\alpha_t P_\phi \overset{\text{def}}{=} U_t P_\phi U_t^* = P_{U_t\phi}$ $\quad (U_t := e^{-iHt},\ \hbar = 1)$

Estimate: $M' = \left| tr(BP_\psi) - tr(BP_\varphi) \right|$

Notation: $\varphi = \phi_t = U_t \phi$, $\psi = U_t V \phi$.

Lemma: $M' \leq \left(\|\psi\| + \|\varphi\| \right) \| B(\psi - \varphi) \|$

$\operatorname{supp} B \subset Y$
$\Rightarrow B = \chi_Y B \chi_Y$

Using the lemma above, we obtain

$M \leq c \| \chi_Y U_t (V\phi - \phi) \|$; $\phi^V = V\phi - \phi$ is supp. in X,
$V = e^A$, $\operatorname{supp} A \subset X$.
bdd

WTS: $\phi^V = (e^A - \mathrm{Id})\phi$ supp. in X.

Indeed,

$$\phi^V := (e^A - \mathrm{Id})\phi = \sum_{n=1}^{\infty} \frac{1}{n!} A^n \phi$$

$$\operatorname{supp} A \subset X \Leftrightarrow A = \chi_X A \chi_X \Rightarrow \chi_{X^c} \phi^V = 0.$$

Upshot: $M \leq c \| \chi_Y U_t \phi^V \| \overset{LCB}{\leq} c\, d_{XY}^{-n} \quad \forall t \leq \frac{d_{XY}}{c}$.

Evaluate

$$\| \chi_Y U_t \phi^V \|^2 = \langle \chi_Y U_t \phi^V, \chi_Y U_t \phi^V \rangle$$

$$= \langle U_t \phi^V, \chi_Y^2 U_t \phi^V \rangle$$

$$= \langle \phi_t^V, \chi_Y^2 \phi_t^V \rangle$$

$$= \operatorname{tr}\left(\chi_Y^2 P_{\phi_t^V} \right)$$

$$\alpha_t(P_\phi) = P_{U_t\phi} \quad = \mathrm{tr}\left(x_y^2\, \alpha_t(P_{\phi_V})\right) \overset{LCB}{\leq} c\, d_{x_y}^{-n}.$$

$\blacksquare$

Lemma: $M' \leq \left(\|\psi\| + \|\varphi\|\right)\|B(\psi-\varphi)\|$

Pf: $M' = |\langle\psi, B\psi\rangle - \langle\varphi, B\varphi\rangle|$

$$\leq |\langle\psi-\varphi, B\psi\rangle| + |\langle\varphi, B(\psi-\varphi)\rangle|$$

Assume $B = B^*$

$$= |\langle B(\psi-\varphi), \psi\rangle| + |\langle\varphi, B(\psi-\varphi)\rangle|$$

Cauchy-Schwartz $\rightarrow$ $\leq \|B(\psi-\varphi)\|\,\|\psi\| + \|\varphi\|\,\|B(\psi-\varphi)\|.$

$\square$

Obs: For rank-1 projections $\sqrt{P_\phi} = P_\phi$. $\leftarrow$ Not true in general for every density op.