QUANTUM DYNAMICS

Consider $H \in \mathcal{L}(\mathcal{H})$, $H = H^*$ and the Schrödinger equation

$$\begin{cases} i\partial_t \psi = H\psi \\ \psi(0) = \psi_0 \in \mathcal{H} \end{cases}$$

We want to study the dynamics of this equation

Rem In this case one can check that $e^{-itH}\psi_0$ is the only solution, with

$$e^{-itH} := \sum_k \frac{(-itH)^k}{k!}$$ as convergent op.

However this def does not extend to unbounded ops

I will make a construction of the propagator via spectral theorem, which extends also to unbounded operators.

Idea: Define the solution via continuous functional calculus

$$U(t)\psi_0 := \phi(e^{-it\lambda})\psi_0 \qquad \forall t$$

↳ via continuous functional calculus

$$e^{-it\lambda} \in C(\sigma(A))$$

Thm $U(t)$ fulfills:

(1) $U(t)$ is a 1-parameter semigroup, unitary, strongly continuous in time

$$U(0) = \mathbb{1}, \quad U(t+s) = U(t)U(s), \quad U(t)^* U(t) = \mathbb{1}$$

$$U(s)\psi \xrightarrow{s \to t} U(t)\psi \quad \text{in } \mathcal{H}$$

(2) $$A\psi := i \lim_{t \to 0} \frac{U(t)\psi - \psi}{t} = i \left.\frac{d}{dt}\right|_{t=0} U(t)\psi$$

(lim in the strong topology)

(3) $\psi(t) := U(t)\psi_0$ is the unique sol of

$i\partial_t \psi = H\psi$ with initial datum ψ_0

proof (1) $H = H^* \rightsquigarrow \sigma(H) \subseteq \mathbb{R}$, then the function $f_t(\lambda) := e^{-it\lambda} \in C(\sigma(A))$ fulfills

$$\overline{f_t(\lambda)}\, f_t(\lambda) = \mathbb{1} \qquad \Phi(f_t(A))^* \Phi(f_t(A)) = \mathbb{1}$$

$$f_t(\lambda)\, f_s(\lambda) = f_{t+s}(\lambda) \quad \Rightarrow \quad \Phi(f_t(A))\,\Phi(f_s(A)) = \Phi(f_{t+s}(A))$$

func. calculus

$$\rightsquigarrow \quad U(t)^* U(t) = \mathbb{1}, \quad U(t)U(s) = U(t+s)$$

Then, to prove strongly continuity: note that

$$\| U(t)\psi - U(s)\psi \|^2 = \| (U(t)-U(s))\psi \|^2$$

$U(t) - U(s)$
$\shortparallel$
$\phi(e^{-it\lambda} - e^{-is\lambda})$
and prop. of

$$= \langle (U(t)-U(s))^* (U(t)-U(s))\psi, \psi \rangle$$

$$= \langle \phi(\overline{f_t - f_s})\, \phi(f_t - f_s)\psi, \psi \rangle$$

$$= \int |f_t - f_s|^2 \, d\mu^H_\psi(\lambda)$$

$$= \int | e^{-it\lambda} - e^{-is\lambda} |^2 \, d\mu^H_\psi(\lambda) \xrightarrow{s \to t} 0$$

by leb dominated convergence theorem

(2) $$\left\| i \left(\frac{U(t) - \mathbb{1}}{t} - A \right) \psi \right\|^2 =$$

$$= \int \left| i \frac{e^{-it\lambda} - 1}{t} - \lambda \right|^2 d\mu^H_\psi(\lambda)$$

Now note that $\left| i \frac{e^{-it\lambda} - 1}{t} - \lambda \right| \xrightarrow{t \to 0} 0$

and $\left| i \frac{e^{-it\lambda} - 1}{t} - \lambda \right| \leq \left| i \frac{e^{-it\lambda} - 1}{t} \right| + |\lambda|$

$$\leq 2|\lambda| \qquad \forall t$$

Again we apply leb dom conv thm and pass to limit

(3) $$\frac{d}{dt} \underbrace{U(t)\psi_0}_{\psi(t)} = \lim_{\varepsilon \to 0} \frac{U(t+\varepsilon)\psi - U(t)\psi}{\varepsilon}$$

$$= \lim_{\varepsilon \to 0} \frac{U(t)\, U(\varepsilon)\psi - U(t)\psi}{\varepsilon} = U(t) \lim_{\varepsilon\to 0} \frac{U(\varepsilon)\psi - \psi}{\varepsilon}$$

$$= \frac{1}{i} U(t)\, A\psi = \frac{1}{i} A \underbrace{U(t)\psi}_{\psi(t)}$$

and $U(0)\psi_0 = \psi_0$ $\rightsquigarrow$ it solves the SE

$\square$

Rem From the proof it is clear that it works $\forall \psi$ in

$$D(H) := \left\{ \psi \in \mathcal{H} : \int \lambda^2 \, d\mu_\psi^H < +\infty \right\}$$

There is also a converse thm

Thm (Stone) Let $U(t)$ a 1-param semigroup, unitary and strongly continuous, then $\forall \psi$ in a dense set,

$$\exists \; i \lim_{t\to 0} \frac{U(t)\psi - \psi}{t} =: A\psi$$

with A a selfadjoint op (in general unbounded) and the solution of $\begin{cases} i\partial_t \psi = A\psi \\ \psi(0) = \psi_0 \end{cases}$ is $U(t)\psi_0$

QUALITATIVE PROPERTIES OF DYNAMICS

$$\begin{cases} i\partial_t \psi = H\psi \\ \psi(0) = \psi_0 \end{cases}$$

Can we say more about the dynamics of Schrödinger equation? As $U(t)$ is unitary

$$\| U(t)\psi_0 \|^2 = \langle \underbrace{U(t)^* U(t)}_{= \mathbb{1}} \psi_0, \psi_0 \rangle = \|\psi_0\|^2 \quad \forall t$$

So the H- norm is preserved by the dynamic.

Moreover if λ_0 is an eigenvalue: $Hu = \lambda_0 u$
then

$$U(t)u = \phi(e^{-itA})u = e^{-it\lambda_0} u$$

$f(A)u = f(\lambda_0)u$

So the evolution is just a rotation!
What about initial data (states) which are orthogonal to eigenvectors?

It is useful to have a new decomposition of the spectrum

Def Let μ be a Borel measure on $\mathbb{R}$. We say

(i) μ is a pure point measure when $\forall M$ Borelian

$$\mu(M) = \sum_{x \in M} \mu(\{x\})$$

(ii) μ is continuous if $\forall x \in \mathbb{R}$, $\mu(\{x\}) = 0$

(iii) μ is absolutely continuous w.r.t. to Lebesgue if

$$|M| = 0 \Rightarrow \mu(M) = 0$$

(iv) μ is singular w.r.t. Lebesgue if $\exists$ Borelian set S with

$$\mu(S) = 0 \quad \text{and} \quad |\mathbb{R} \setminus S| = 0$$

μ and μ_{Leb} supported on different sets

Thm 1 (Lebesgue–Radon–Nikodym) Any measure μ on $\mathbb{R}^n$ can be written in a unique way as

$$\mu = \mu_{ac} + \mu_{sing}$$

where μ_{ac} is a.c. w.r.t. Lebesgue
μ_{sing} " singular " "

Moreover, $\exists!\ h \in L^1(\mu_{Leb})$ s.t. $\mu(E) = \int_E h \, d\mu_{Leb}$ ← Radon Nikodym
$\forall\ E$ Borel set.

proof Rudin, "Real and complex analysis", Thm 6.10
(apply with $\mu \equiv \mu_{Leb}$, $\lambda \equiv \mu$)

Now let μ a Borel measure on $\mathbb{R}$.
We can decompose it also as

(*) $$\mu = \mu_{pp} + \mu_{cont}$$ with μ_{pp} pure point, μ_{cont} continuous

Indeed put $P = \{ x \mid \mu(\{x\}) \neq 0 \}$. Since μ is Borel, P is a countable set (use $\mu(K) < +\infty$ $\forall$ K compact set). Put

$$\mu_{pp}(M) := \sum_{x \in M \cap P} \mu(\{x\}) = \mu(P \cap M)$$

One checks that
- μ_{pp} is a pure point measure
- $\mu_{cont} := \mu - \mu_{pp}$ is positive
- $\mu_{cont}(\{x\}) = 0$ $\forall$ x

So take μ finite Borel measure, apply Lebesgue to get

$$\mu = \mu_{ac} + \mu_{sing} \quad , \quad \text{then apply } (\neq) \text{ to } \mu_{sing} : \text{ we get}$$

Thm (Lebesgue decomposition thm) Let μ be a Borel measure on $\mathbb{R}$. Then one has the unique decomposition

$$\mu = \mu_{ac} + \mu_{pp} + \mu_{sc} \qquad \text{where}$$

μ_{ac} : absolutely continuous w.r.t. Lebesgue

μ_{pp} : pure point measure

μ_{sc} : is singular w.r.t. Lebesgue and continuous.

EXAMPLE : $\mu_{pp} = \sum a_n \delta_{x_n}$ (Dirac's delta centered at x_n)

μ_{sc} : Let F be the Cantor function defined on the Cantor set:

It is continuous but not absolutely continuous, and $|\text{Cantor set}| = 0$.

Define the measure

$$\mu_{sc}((a,b]) = F(b) - F(a) \qquad \text{interval}$$

$$\mu_{sc}(M) = \inf \left\{ \sum_k \mu_{singc}(J_k) \ : \ \begin{array}{l} J_k \text{ half open interval} \\ \cup J_k \supseteq M \end{array} \right\}$$

for a Borel set M.

Then μ_{singc} is singular w.r.t. Lebesgue

Application: $A \in \mathcal{L}(\mathcal{H})$, $A = A^*$, then $\forall x \in \mathcal{H}$

$$\mu_x^A = \mu_{x,ac}^A + \mu_{x,pp}^A + \mu_{x,sc}^A$$

Accordingly, we put

$$\begin{aligned}
\mathcal{H}_{pp} &= \{ x \in H \mid \mu_x \text{ is } pp \} \\
\mathcal{H}_{ac} &= \{ x \in H \mid \mu_x \text{ is } ac \} \\
\mathcal{H}_{sc} &= \{ x \in H \mid \mu_x \text{ is } sc \} \\
\mathcal{H}_{c} &= \{ x \in H \mid \mu_x \text{ is continuous} \}
\end{aligned}$$

If sets are empty, put $\{0\}$.

Thm $\mathcal{H} = H_{pp} \oplus H_{ac} \oplus H_{sc}$, closed, orthogonal subspaces, invariant by A

Def (Decomposition of spectrum)

$\boxed{\text{⚠ DIFFERENT BOOKS DIFFERENT NOTATIONS}}$

$$\sigma_{pp}(A) = \{ \lambda \mid \lambda \text{ eigenvalue of } A \},$$

$$\sigma_c(A) = \sigma\left(A|_{\mathcal{H}_{ac} \oplus \mathcal{H}_{sc}} \right)$$

$$\sigma_{ac}(A) = \sigma\left(A|_{\mathcal{H}_{ac}} \right), \quad \sigma_{sc}(A) = \sigma\left(A|_{\mathcal{H}_{sc}} \right)$$

Prop

$$\sigma(A) = \underbrace{\overline{\sigma_{pp}(A)}}_{= \sigma(A|_{\mathcal{H}_{pp}})} \cup \sigma_c(A)$$

composed by eigenvalues of A and its accumulation points

$$\sigma_c(A) = \sigma_{ac}(A) \cup \sigma_{sc}(A)$$

proof (theorem) (1) We first prove that

$$H_{pp} = \overline{\operatorname{span}\{ \psi \in H \mid \psi \text{ eigenvectors} \}}$$

$(\supseteq)$ $\psi = \sum_n \psi_n$ with $A\psi_n = \lambda_n \psi_n$, λ_n eigenvalue

Then $E^A(\cup\{\lambda_n\})\psi = \sum_m E^A(\cup\{\lambda_n\})\psi_m = \sum_{m,n} E^A(\{\lambda_n\})\psi_m$

$E^A(\{\lambda_n\}) = P_{\ker(A-\lambda_n)}$

$= \sum_n E^A(\{\lambda_n\})\psi_n = \psi$

Hence $\mu^A_\psi(\Omega) = \langle E^A(\Omega)\psi,\psi\rangle = \langle E^A(\Omega)E^A(\cup\{\lambda_n\})\psi,\psi\rangle$

$= \sum_{x\in\Omega\cap\cup\{\lambda_n\}} \mu^A_\psi(\{x\})$

$(\subseteq)$ Let $\psi \in H_{pp}$. Then μ^A_ψ supported in countable set $N = \bigcup_n \{\eta_n\}$ $\Rightarrow$ $\psi \in \operatorname{Im} E^A(N)$

$\Rightarrow \psi = E^A(N)\psi = \sum E^A(\{\eta_n\})\psi$

Put $\psi_n := E^A(\{\eta_n\})\psi$. We show it is eigenvector

$\|(A-\eta_n)\psi_n\|^2 = \int(\lambda-\eta_n)^2\, d\mu^A_{\psi_n} = 0$

In particular H_{pp} is closed Hilbert space in H.

(2) We check that $H_c = H_{pp}^\perp$

$(\supseteq)$ Let $\psi \in H_{pp}^\perp$. For $\lambda\in\mathbb{R}$, put $\psi_\lambda := E^A(\{\lambda\})\psi \in \ker(A-\lambda)$ then

$0 = \langle\psi_\lambda,\psi\rangle = \langle E^A(\{\lambda\})\psi,\psi\rangle = \mu^A_\psi(\{\lambda\})$

either $\psi_\lambda \neq 0 \in H_{pp}$ and $\psi \perp H_{pp}$

or $\psi_\lambda = 0$ (recall $E^A(\{\lambda\}) \neq 0 \Leftrightarrow \lambda\in\sigma_{pp}(A)$)

$(\subseteq)$ $\psi\in H_c$ and ψ_n eigenvector, $A\psi_n = \lambda_n\psi_n$.

then $E^A(\{\lambda_n\})\psi_n = \psi_n$, and

$$|\langle\psi,\psi_n\rangle| = |\langle\psi, E^A(\{\lambda_n\})\psi_n\rangle| \leq \underbrace{|\langle E^A(\{\lambda_n\})\psi,\psi\rangle|}_{=0}^{1/2} \times \underbrace{|\langle E^A(\{\lambda_n\})\psi_n,\psi_n\rangle|}_{\|\psi_n\|}^{1/2}$$

(3) We consider $H_{ac} \subseteq H_c$. We show that H_{ac} is closed subspace.

Let $(\psi_n)_{n\geq 1} \subseteq H_{ac}$, $\psi_n \to \psi$ in $\mathcal{H}$.

Let Ω be measurable set with $|\Omega| = 0$, want to show $\langle E^A(\Omega)\psi,\psi\rangle = 0$.

As $\langle E^A(\Omega)\psi,\psi\rangle = \lim_{n\to\infty} \langle E^A(\Omega)\psi, \psi_n\rangle$, enough to show that $\langle E^A(\Omega)\psi, \psi_n\rangle = 0$ $\forall n$. But

$|\langle E^A(\Omega)\psi, \psi_n\rangle| = |\langle E^A(\Omega)\psi, E^A(\Omega)\psi_n\rangle| \leq \|E^A(\Omega)\psi\|^{1/2} \underbrace{\|E^A(\Omega)\psi_n\|^{1/2}}$

$\psi_n \in H_{ac}$ $\qquad \langle E^A(\Omega)\psi_n, \psi_n\rangle = 0$ $\forall n$

(4) We show $H_{sc} = H_{ac}^{\perp_{H_c}}$. Clearly it is closed.

($\subseteq$) Let $\psi \in H_{sc} \Rightarrow \mu^A_\psi$ is sing cont

$\rightsquigarrow \exists$ set M with $\mu^A_\psi(M) \neq 0$ & $|M| = 0$

Then $\psi = E^A(M)\psi$ and $\forall$ $\varphi \in H_{ac}$

$\langle \psi, \varphi\rangle = \langle E^A(M)\psi, \varphi\rangle = \langle \psi, \underbrace{E^A(M)\varphi}_{=0}\rangle = 0$

($\supseteq$) Let $\psi \in H_{ac}^{\perp_{H_c}}$. Decompose $\mu^A_\psi = \mu^A_{\psi,pp} + \mu^A_{\psi,ac} + \mu^A_{\psi,sc}$

$\psi \in H_c \Rightarrow \mu^A_{\psi,pp} = 0$

$\psi \in H_{ac}^{\perp} \Rightarrow \mu^A_{\psi,ac} = 0$ $\qquad \rightsquigarrow \mu^A_\psi$ is sing. cont

Indeed: P.A. $\mu^A_{\psi,ac} \neq 0$, hence $\exists$ set N with $\mu^A_{\psi,ac}(N) \neq 0$

but $\mu^A_{\psi,sc}(N) = 0$. then $\mu^A_\psi(N) = \mu^A_{\psi,ac}(N) \neq 0$

so ·) $E^A(N)\psi \neq 0$

·) $E^A(N)\psi \in H_{ac}$. Indeed if $|\Omega| = 0$, then

$\mu^A_{E^A(N)\psi}(\Omega) = \langle E^A(N\cap\Omega)\psi,\psi\rangle = \mu^A_\psi(N\cap\Omega) = \mu^A_{\psi,ac}(N\cap\Omega) = 0$

$\rightsquigarrow 0 \neq \|E^A(N)\psi\|^2 = \langle \underbrace{E^A(N)\psi}_{\in H_{ac}}, \underbrace{\psi}_{\in H_{ac}^{\perp}}\rangle = 0$ $\lightning$

Application to dynamics

Thm $A \in \mathcal{L}(H)$, $A = A^*$, K compact op. then

$\boxed{\text{RAGE THM}}$

(1) $\forall \varphi \in H_c$: $\displaystyle\lim_{T \to +\infty} \frac{1}{T} \int_0^T \| K e^{-itA} \varphi \|^2 dt = 0$

(2) $\forall \varphi \in H_{ac}$: $\displaystyle\lim_{t \to +\infty} \| K e^{-itA} \varphi \| = 0$

proof K compact, H Hilbert $\rightsquigarrow$ approximate K by finite ranks K_n

$$\rightsquigarrow \quad \| K e^{-itA} \varphi \| \leq \| K_n e^{-itA} \varphi \| + \underbrace{\|(K - K_n)\|}_{\to 0} \underbrace{\| e^{-itA} \varphi \|}_{= \|\varphi\|}$$

So enough to prove the results for $K_n e^{-itA} \varphi$

Moreover $K_n = \sum_{\ell=1}^{N(n)} \eta_\ell \langle \cdot , x_\ell \rangle$ with $\eta_\ell, x_\ell \in H$.

Then

$$\| K_n e^{-itA} \varphi \| \leq \sum \| \eta_\ell \| \, | \langle e^{-itA} \varphi, x_\ell \rangle |$$

so enough to prove

$\displaystyle\frac{1}{T} \int_0^T | \langle e^{-itA} \varphi, x_\ell \rangle |^2 dt \to 0 \quad \forall \varphi \in H_c$, $\langle e^{-itA} \varphi, x_\ell \rangle \xrightarrow{t \to +\infty} 0 \quad \forall \varphi \in H_{ac}$

By spectral thm $\displaystyle \langle e^{-itA} \varphi, x_\ell \rangle = \int e^{-it\lambda} d\mu^A_{\varphi, x_\ell}$

(1) $\varphi \in H_c \Rightarrow \mu^A_{\varphi, x_\ell}$ is continuous measure. Then apply

Thm (Wiener) μ finite complex Borel measure on $\mathbb{R}$

$$\hat{\mu}(t) := \int_{\mathbb{R}} e^{-it\lambda} d\mu(\lambda).$$

Then

$$\lim_{T \to +\infty} \frac{1}{T} \int_0^T | \hat{\mu}(t) |^2 dt = \sum_{\lambda \in \mathbb{R}} | \mu(\{\lambda\}) |^2$$

by very def. $\hat{\mu}(t) = \langle e^{-itA}\varphi, \chi_\ell\rangle$, thus Wiener

$$\frac{1}{T}\int_0^T |\langle e^{-itA}\varphi, \chi_\ell\rangle|^2 \longrightarrow \sum_{\lambda\in\mathbb{R}} \underbrace{|\mu^A_{\varphi,\chi_\ell}(\{\lambda\})|^2}_{=0}$$

(2) $\varphi \in H_{ac} \Rightarrow \mu^A_{\varphi,\chi_\ell}$ is a.c.

$$|\mu^A_{\varphi,\chi_\ell}(\Omega)| = |\langle E^A(\Omega)\varphi, \chi_\ell\rangle| \leq \|E^A(\Omega)\varphi\|^{1/2}\,\|\chi_\ell\|^{1/2}$$
$$\leq \mu^A_\varphi(\Omega)^{1/2}\,\|\chi_\ell\|^{1/2}.$$ Hence $|\Omega| = 0 \Rightarrow \mu^A_\varphi(\Omega) = 0$
$\Rightarrow \mu^A_{\varphi,\chi_\ell}(\Omega) = 0$

Radon-Nikodym: $\mu^A_{\varphi,\chi_\ell} = f(\lambda)\, d\mu_{Leb}$, $f \in L^1$.

Riemann-Lebesgue lemma: $\int e^{-it\lambda} f(\lambda)\, d\mu_{Leb} \xrightarrow{t\to+\infty} 0$ $\square$