QUANTUM MECHANICS COURSE NOTES

~~M 1-230 WB 1441~~ M 1-4 BA 1240
~~W 1-230 BA 2145~~

Sources

[J: QM] R. Jerrard's Quantum Mechanics Course notes: APM421 2005

[wiki: MFQM] Wikipedia: Mathematical Foundations of Quantum Mechanics

[GS] Gustafson - Sigal

[vN: MFQM] J. von Neumann: Math. Foundations of QM

[RszN: FA] Riesz - Sz. Nagy: Functional Analysis

[H: QM] K. Hannabuss: Intro to Quantum Theory

[LL: Classical Fields] Landau - Lifschitz: theory of classical fields

[N] R. C. Newburgh "The ... Bugler relations as Lorentz invariants" (article)

[J : QM] p5, 8-10

$\boxed{\text{SPECTRAL THEOREM}}$ $\forall$ $A : \mathbb{H} \to \mathbb{H}$, $\langle Af, g \rangle = \langle f, Ag \rangle$ $\forall f, g \in \mathbb{H}$

$\exists!$ spectral family of orthogonal projection operators $\{E_\lambda\}_{\lambda \in \mathbb{R}}$:

A self-adjoint

Ingredients :
• Hilbert space $\mathbb{H}$
• operator $A : \mathbb{H} \to \mathbb{H}$
$\rightsquigarrow \{E_\lambda\}$

- $E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda$ for $\lambda \le \mu$
- $E_\lambda = \underset{\mu \searrow \lambda}{\text{s-lim}}\ E_\mu$
- $\underset{\lambda \searrow -\infty}{\text{s-lim}}\ E_\lambda = 0$; $\underset{\lambda \to +\infty}{\text{s-lim}}\ E_\lambda = \mathbb{1}$.

and

$$A = \int_{-\infty}^{\infty} \lambda \, dE_\lambda = \underset{N \to \infty}{\text{s-lim}} \int_{-N}^{N} \lambda \, dE_\lambda$$

$$D(A) \doteq \{ \psi \in \mathbb{H} : \int_{-\infty}^{\infty} \lambda^2 \, d\langle \psi, E_\lambda \psi \rangle < \infty \}$$

We will soon collect the terminology required to understand the statement. We first consider some examples...

<u>Finite-d example</u> $\mathbb{H} = \mathbb{C}^n$; $\langle f, g \rangle = \overline{(\ f\ )}\begin{pmatrix} g \end{pmatrix} = \sum_{i=1}^{n} \bar{f}_i g_i$

$A : \mathbb{H} \to \mathbb{H}$; $\langle Af, g \rangle = \langle f, Ag \rangle$

Principal axis theorem

linear algebra $\Longrightarrow$

- $\exists$ ONB of eigenvectors $\{v_1, \dots, v_n\}$ of $\mathbb{C}^n$:

  $A v_j = \lambda_j v_j$ (eigenvalues w. multiplicity)

  $\langle v_j, v_k \rangle = \delta_{jk}$
- A is determined by its eigenvectors and eigenvalues :

  $$A w = \sum_{i=1}^{n} \langle v_i, w \rangle \lambda_i v_i \qquad \forall w \in \mathbb{H}.$$

spectral family $\forall j$ $P_j : \mathbb{H} \to \text{span}(v_j)$ so $P_j w = \langle v_j, w \rangle v_j$

$$E_\lambda = \sum_{\{j : \lambda_j \le \lambda\}} P_j$$

Exercise: Justify
$\{E_\lambda\}_{\lambda \in \mathbb{R}}$ is spectral family

<u>∞-d example</u> (Discrete Spectrum)

$\mathbb{T} = \mathbb{R}/\mathbb{Z}$. $\quad \mathcal{H} = L^2(\mathbb{T}) = \{ f : (0,1) \to \mathbb{C} \mid f(0) = f(1) ; \ \langle f, f \rangle < \infty \}$

$$\langle f, g \rangle = \int_0^1 \bar{f}(x)\, g(x)\, dx \quad ; \quad dx \text{ Lebesgue.}$$

A self-adjoint.

$D(A) = \{ \psi \in \mathcal{H} \mid \psi' \in \mathcal{H} \}$

$A\psi := i\psi'$; verify self-adjointness via IBP.

$e_j(x) = e^{-2\pi i j x}$, $\quad j \in \mathbb{Z}$. $\qquad A e_j = \underbrace{(2\pi j)}_{\lambda_j} e_j$

Harmonic Analysis $\Longrightarrow$ $\{e_j\}_{j=-\infty}^{\infty}$, ONB of $L^2(\mathbb{T})$.

Eigenspace projection sum representation:

$$A\psi = \sum_{j=-\infty}^{\infty} \langle e_j, \psi \rangle \lambda_j e_j \quad , \quad \forall \ \psi \in D(A).$$

spectral family representation:

$\boxed{\text{Exercise: Justify....}}$

$$P_j w = \langle e_j, w \rangle e_j$$

$$E_\lambda := \sum_{\{j : \lambda_j \le \lambda\}} P_j$$

<u>∞-d example</u> (cts. spectrum)

$\mathbb{H} = L^2(\mathbb{R}) = \{ \psi : \mathbb{R} \to \mathbb{C} \mid \langle \psi, \psi \rangle < \infty \}$; $\langle f, g \rangle = \int_{\mathbb{R}} \bar{f}(x)\, g(x)\, dx$.

$D(A) = \{ \psi \in \mathbb{H} \mid \int_{\mathbb{R}} x^2 |\psi(x)|^2 dx < \infty \}$

$A\psi(x) = x\psi(x)$

A has no eigenfunctions/eigenvalues: $\forall \lambda \in \mathbb{R}$ $\nexists \psi \in \mathbb{H}$ s.t. $A\psi = \lambda\psi$.

Thus, eigenspace projection representation is unsuitable for A.

$\forall$ $\lambda \in \mathbb{R}$ define $E_\lambda : \mathbb{H} \to \mathbb{H}$ by $(E_\lambda \psi)(x) = \begin{cases} \psi(x) & \text{if } x \le \lambda \\ 0 & \text{otherwise} \end{cases}$.

Thus, $E_\lambda f(x) = M_\lambda(x) f(x)$ with $M_\lambda(x) = \begin{cases} 1 & \text{if } x \le \lambda \\ 0 & \text{otherwise}. \end{cases}$

<u>Exercise</u>: Verify $\{E_\lambda\}_{\lambda \in \mathbb{R}}$ is a spectral family for A.

<u>Special Relativistic Motivation for de Broglie's relations</u> LL: [illegible], [V]

Consider a (pure, monochromatic) wave $\psi(t,\underline{x}) = e^{-i(\omega t - \underline{k}\cdot\underline{x})}$ with temporal [LL], [V]
frequency ω and spatial wave vector $\underline{k}$. The parameters $\underline{k}$ and ω encode the
oscillation properties of this pure wave. In his theory of black body radiation,
Planck associated the notion of energy to a wave with his relation $E = \hbar\omega$.
Later, Einstein, in his theory of the photoelectric effect, demonstrated the usefulness
of this energy-frequency relationship.

Unfortunately, the Planck relation $E = \hbar\omega$ is inconsistent with special relativity. This
inconsistency led de Broglie to a more general relationship spawning a link
with momentum and the wave vector $\underline{k}$.

Special relativity is a description of spacetime as a collection of events $(t, \underline{x})$
with an absolute upper bound on velocities given by the speed of light c. The
invariance of the speed of light is encoded in the theory by the demand that
physical relationships among events must be invariant under Lorentz transformations.
A Lorentz transformation $\Lambda : \mathbb{R}^{1+4} \to \mathbb{R}^{1+4}$ is a map $(t,x) \to (\Lambda t, \Lambda x)$
which leaves the Lorentz metric $ds^2 = -c^2 dt^2 + dx_1^2 + dx_2^2 + dx_3^2$. (These can
be classified.) Anyway, it can be shown that the phase $(\omega t - \underline{k}\cdot\underline{x})$ of
the pure wave is Lorentz invariant: $(\omega t - \underline{k}\cdot\underline{x}) = (\omega\Lambda t - \Lambda\underline{k}\cdot\Lambda\underline{x})$.
However, the time-frequency is not invariant $\omega \neq \Lambda\omega \quad \forall\ \Lambda \in \{\text{Lorentz}\}$.
Since energy is a physical quantity, we encounter a troubling inconsistency since
the Planck relation $E = \hbar\omega$ is not Lorentz invariant.

The resolution of the inconsistency involves enlarging our viewpoint to account for
the relativistic links between space and time. The wave 4-vector $(\frac{\omega}{c}, k) = \mathbb{K}$
is relativistically invariant. Prior to Lorentz transformation, the Planck relationship
is a statement about the 1st component of $\mathbb{K}$. L. de Broglie observed
that the momentum 4-vector $\mathbb{P} = (E/c, \underline{p})$ is also a Lorentz invariant
and argued we should extend the Planck relationship by writing $\mathbb{K} \propto \mathbb{P}$.
Thus, wave properties encoded in the wave 4-vector $\mathbb{K}$ are associated with
classical mechanics particle notions encoded in $\mathbb{P}$. The Planck relation identifies
the constant of proportionality between these parallel 4-vectors: $\hbar$!

We thus obtain the de Broglie formula $\underline{p} = \hbar\underline{k}$ linking momentum to wave vector.

Motivation for Schrödinger's Equation [Hannabuss, 5-6]

Planck, Einstein observed that the energy and frequency of light are related by formula $E = \hbar\omega$. De Broglie observed that to be consistent w. relativity, the momentum $\underline{p}$ of a wave should be $\underline{p} = \hbar \underline{k}$ where $\underline{k}$ is the wave vector of magnitude $2\pi/\text{wavelength}$, perpendicular to the wave front.

Explain special relativity $\rightarrow$ de Broglie's idea

With this dictionary, wave properties $(\omega, \underline{k})$ are linked with dynamical constructs from physics $(E, \underline{p})$. Schrödinger's idea was to relax to considering more general waves, namely waves without a well-defined wave vector $\underline{k}$ or frequency ω and to then extract the physical notions of Energy and momentum from the wave by some other means.

de Broglie relations

Consider a plane wave $\psi(t,x) = e^{-i(\omega t - \underline{k}\cdot\underline{x})}$ of frequency ω and wave vector $\underline{k}$. What do we have to "do" to ψ to "get" the energy $E = \hbar\omega$? Well, we apply the operator $i\hbar\partial_t$: $i\hbar\partial_t\psi = \hbar\omega\cdot\psi$. Similarly, when we apply the operator $\frac{\hbar}{i}\nabla$ to the plane wave, we obtain the momentum $\underline{p}$: $\frac{\hbar}{i}\nabla\psi = \hbar k\,\psi$.

Since there exist waves other than plane waves (for which $\omega, \underline{k}$ are well-defined constants) and general waves do not have well-defined frequency ω or well-defined wave vector, we need some other way to attach the energy and momentum to a general wave. We generalize the Planck-Einstein Energy-frequency relation for plane waves by defining $E\psi = i\hbar\partial_t\psi$. We generalize the de Broglie wave-vector momentum relation for plane waves by writing $\underline{p}\psi = \frac{\hbar}{i}\underline{\nabla}\psi$.

A particle of mass m in potential well given by $V(x)$ has energy:

$$E = \frac{|\underline{p}|^2}{2m} + V(x) \underset{\text{translate}}{\longleftrightarrow} i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi + V\psi.$$

Physical Motivation for Schrödinger Equation

Experiments (e.g. double slit) and other sources (e.g. theory) have led to the idea that physical systems (e.g. electron, hydrogen atom, semiconductors, ...) are described by a <u>wave function</u>: $\psi : [0,T) \times \mathbb{R}^d \to \mathbb{C}$. <u>Consider one particle case</u>

- $|\psi(t,\cdot)|^2$ is probability distribution for particle's position

  e.g. $\text{Prob}(\text{particle in } \Omega \subset \mathbb{R}^3 \text{ at time } t) = \int_\Omega |\psi(t,x)|^2 dx$.

- ψ satisfies some sort of wave equation.

OK, if we take this seriously, we should mathematize it, make it rigorous, investigate logical consequences, build things with the emerging ideas ...

We need to
- determine the equation satisfied by ψ;
- Solve and study that equation;
- Give descriptions of the solution;
- . . .

[GS; 4-5]

What is the equation that ψ satisfies? Among all possible equations, we select an equation by identifying physically reasonable criteria the equation should satisfy and then we make a choice.

<u>Criteria for Wave Equation</u>

- (Causality/Determinism) $\psi(t_0,x)$, $x \in \mathbb{R}^d$ should determine $\psi(t,x)$ $\forall t > t_0$.
- (Linearity) ψ, ϕ physical "solutions" solutions then $\alpha\psi + \beta\phi$ is also a solution.
- (Classical Correspondence) Under normal human scale conditions, physics described by ψ should correspond with classical physics.

{ We could impose other natural criteria. Or we could make a choice based on these principles. Let's see how these narrow things down ...

Causality/Determinism suggests our equation should be <u>first order in time</u>. Let's look for equation of the form $\frac{\partial}{\partial t}\psi = A\psi$ for some A acting on our space of solutions. We restrict to A being <u>linear</u> <u>operators</u> acting on the state space. "Vector field equation on state space."

What is the form of the operator A? We select the form of A in correspondence with the <u>classical</u> <u>Hamilton-Jacobi equation</u> and an associated high frequency approximation, the <u>eikonal equation</u>.

Classical Inputs:

- A fundamental equation of first-order-in-time from classical mechanics links the classical action $S(t,x)$ with the classical hamiltonian $h(t,x)$: (Hamilton - Jacobi Equation)

HJ $$\frac{\partial}{\partial t} S = -h(x, \nabla_x S).$$

The hamiltonian is often of the form: $h(x,k) = \frac{|k|^2}{2m} + V(x)$ where m is mass, V is the potential. (The relevance of HJ to classical mechanics should! could be further developed.)

- Classical links (to be developed): HJ linked to eikonal equation. High frequency approximation to classical wave equation linked to eikonal equation: for $u = ae^{i\phi}$ satisfying wave equation.

eikonal $$\left(\frac{\partial\phi}{\partial t}\right)^2 - |\nabla_x \phi|^2 = 0$$

We seek the form of the operator A in the (target) wave equation $\partial/\partial t\, \psi = A\psi$ so that it has solutions of the form

$$\psi(t,x) = a(t,x)\, e^{iS(t,x)/\hbar} \qquad (\hbar \ll 1)$$

with S satisfying HJ equation! We assume a, S and their derivatives are order one in $\hbar$. A calculation to leading order in $\hbar$ reveals that ψ satisfies

$LS_V(\mathbb{R}^d)$ $$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\Delta_x\psi + V(x)\psi.$$

We enlarge the discussion to setting of self-adjoint H.

$$:= H\psi.$$

This equation explains physical experiments beyond the classical theory with the choice of $\hbar \simeq 6.0 \times 10^{-27}$ erg./sec (Planck's constant)

The physical situation described by $LS_V(\mathbb{R}^d)$ depends upon the choice of potential V, e.g. $V(x) = -\alpha/|x|$ for hydrogen atom...

Dynamics? Cauchy - Problem or initial - value - problem for $LS_V(\mathbb{R}^d)$:

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

A first basic issue is well-posedness?
After that, describe solutions!
We should also validate consistencies with our motivations and criteria.

Lecture 3

<u>Hilbert space Basics</u>: $\mathbb{H}$ complex vector space with an <u>inner product</u> $\langle \cdot , \cdot \rangle : \mathbb{H} \times \mathbb{H} \to \mathbb{C}$ which satisfies: (i) $\langle v, \alpha w + \beta z \rangle = \alpha \langle v, w \rangle + \beta \langle v, z \rangle$, (ii) $\langle w, v \rangle = \overline{\langle v, w \rangle}$, (iii) $\langle v, v \rangle > 0 \ \forall v \neq 0$ and $\forall v, w, z \in \mathbb{H}$, $\alpha, \beta \in \mathbb{C}$.

The map $\| \cdot \| : \mathbb{H} \to \mathbb{R}$ defined by $\|v\| = \langle v, v \rangle^{1/2}$ is a <u>norm</u> on $\mathbb{H}$.
(i) $\|\alpha v\| = \alpha \|v\|$, (ii) $\|v + w\| < \|v\| + \|w\|$, (iii) $\|v\| > 0 \ \forall v \neq 0$.

The Hilbert space $\mathbb{H}$ is <u>complete</u> in this norm.

Thus, A <u>Hilbert space</u> is a complex vector space which is complete in the norm associated to the inner product.

<u>Examples</u>, $L^2(\mathbb{R}^d) = \{ \psi : \mathbb{R}^d \to \mathbb{C} \mid \int_{\mathbb{R}^d} |\psi|^2 \, dx < \infty \}$, w. $\langle \psi, \phi \rangle = \int_{\mathbb{R}^d} \overline{\psi} \phi \, dx$.

$H^n(\mathbb{R}^d) = \{ \psi \in L^2(\mathbb{R}^d) \mid \partial^\alpha \psi \in L^2(\mathbb{R}^d) \ \forall \alpha, |\alpha| \leq n$ (multiindex) $\}$.

$\left(\alpha = (\alpha_1, \dots, \alpha_d) ; \ \partial^\alpha \psi = \partial_{x_1}^{\alpha_1} \cdots \partial_{x_d}^{\alpha_d} \psi ; \ |\alpha| = \sum_{j=1}^{d} |\alpha_j| . \right)$ w.

$$\langle \psi, \phi \rangle_{H^n} = \sum_{|\alpha| \leq n} \langle \partial^\alpha \psi, \partial^\alpha \phi \rangle .$$

Terminology for Spectral Theorem

All operators for us will be linear: $S(a\psi + b\phi) = a\,S(\psi) + b\,S(\phi)$ $\forall\, a,b \in \mathbb{C}$ $\forall\, \psi,\phi \in \mathbb{H}$. "bounded operator" means "bounded linear operator", etc.

A bounded operator $S : \mathbb{H} \to \mathbb{H}'$ is one which satisfies: $\|S\psi\|_{\mathbb{H}'} \leq C \|\psi\|_{\mathbb{H}}$ for some bounded constant C and for all $\psi \in \mathbb{H}$.

An unbounded operator $A : \mathbb{H} \to \mathbb{H}'$ is an operator from a subspace $D(A) \subset \mathbb{H}$ to $\mathbb{H}'$. The subspace $D(A)$ is called the domain of A and it is a part of the definition of A. If A_1, A_2 are unbounded operators such that $D(A_1) \neq D(A_2)$ but $A_1 = A_2$ on $D(A_1) \cap D(A_2)$ then A_1 and A_2 are different operators.

If $D(A)$ is dense in $\mathbb{H}$ and $\|A\psi\|_{\mathbb{H}} \leq C\|\psi\|_{\mathbb{H}}$ $\forall\, \psi \in D(A)$ then A extends to a unique bounded operator on $\mathbb{H}$. Verify this fact.

An operator A is closed if its graph $\{(\phi, A\phi) \in \mathbb{H} \oplus \mathbb{H} \mid \psi \in D(A)\}$ is closed in $\mathbb{H} \oplus \mathbb{H}$. In other words, A is closed if: $\psi_n \in D(A)$, $\psi_n \to \psi$; $A\psi_n \to \phi \Longrightarrow \psi \in D(A)$ and $A\psi = \phi$.

Null space of A, denoted $N(A) = \{\psi \in D(A) : A\psi = 0\}$.

Range of A, denoted $R(A) = \{A\psi : \psi \in D(A)\}$

An operator A (bounded or unbounded) is one-to-one if $N(A) = \{0\}$.

If A is one-to-one we define A^{-1} by $D(A^{-1}) = R(A)$;
$A^{-1}\psi = \phi \Longleftrightarrow \psi = A\phi$. A is invertible if A^{-1} exists and is bounded.

Operator Adjoints. $A: \mathbb{H} \to \mathbb{H}'$ operator. $D(A)$ dense in $\mathbb{H}$. We define $A^*: \mathbb{H}' \to \mathbb{H}$ by
$D(A^*) = \{\psi \in \mathbb{H}' : \exists\ C < \infty$ s.t. $|\langle \psi, A\phi\rangle_{\mathbb{H}'}| < C\|\phi\|_{\mathbb{H}} \quad \forall\ \phi \in D(A)\}$.
and $A^*\psi$ defined by requiring: $\langle A^*\psi, \phi\rangle_{\mathbb{H}} = \langle \psi, A\phi\rangle_{\mathbb{H}'}, \quad \forall\ \phi \in D(A)$.

Exercise: Verify that $A^*\psi$ is well-defined if $D(A)$ is dense in $\mathbb{H}$.

Examples $\mathbb{H} = L^2([0,1])$ w. standard inner product. [J]

$D(A_1) = \{\psi \in \mathbb{H} : \psi' \in \mathbb{H},\ \psi(0) = \psi(1) = 0\}$

$D(A_2) = \{\psi \in \mathbb{H} : \psi' \in \mathbb{H},\ \psi(0) = \psi(1)\}$

$D(A_3) = \{\psi \in \mathbb{H} : \psi' \in \mathbb{H}\}$.

For $\psi \in D(A_j)$ set $A_j\psi = i\hbar\psi'$, $j = 1, 2, 3$.

Note: $\psi' \in \mathbb{H} \Rightarrow \exists\ \phi \in \mathbb{H}$ and $c \in \mathbb{C}$ s.t. $\psi(x) = c + \int_0^x \phi(s)\,ds$ a.e. x.

We compute adjoints:

$D(A_j^*) = \{\psi \in \mathbb{H} : \exists\ \eta \in \mathbb{H}$ s.t. $\langle \psi, A_j\phi\rangle = \langle \eta, \phi\rangle \quad \forall\ \phi \in D(A_j)\}$

Fix $\psi \in D(A_j^*)$ and let η be as above so that

$$\int_0^1 \bar{\psi}\,(i\hbar\,\phi')\,dx = \int_0^1 \bar{\eta}\,\phi\,dx \qquad \forall\ \phi \in D(A_j). \quad (\text{Thus, } \eta = A_j^*\psi)$$

Let $\zeta(x) = \int_0^x \eta(y)\,dy = \int_0^x A_j^*\psi(y)\,dy$ and $\zeta \in \mathbb{H}$ with $\zeta' = \eta$.

Note $\zeta(0) = 0$. IBP (valid in this setting ...) yields

$$\int_0^1 \bar{\eta}\,\phi\,dx = \int_0^1 \bar{\zeta}'\,\phi\,dx = (\bar{\zeta}\phi)\Big|_0^1 - \int_0^1 \bar{\zeta}\,\phi'\,dx.$$

Thus, we find $\psi \in D(A_j^*)$ if and only if

$$(*) \qquad \int_0^1 (i\hbar\bar{\psi})\,\phi'\,dx = \bar{\zeta}\phi\Big|_0^1 - \int_0^1 \bar{\zeta}\,\phi'\,dx \qquad \forall\ \phi \in D(A_j).$$

Adjoint of A_1: $\phi \in D(A_1) \Rightarrow \phi(0) = \phi(1) = 0$ so $(*)$ reduces to

$$-\int_0^1 \overline{i\hbar\psi}\,\phi'\,dx = -\int_0^1 \bar{\zeta}\,\phi'\,dx \qquad \forall\ \phi \in D(A_1).$$

Claim: $\{\phi' : \phi \in D(A_1)\} = \{f \in \mathbb{H} : \int_0^1 f\,dx = 0\}$ (easy)

Thus, $(*)$ becomes $\int_0^1 \overline{(i\hbar\psi - \zeta)}\,f\,dy = 0 \quad \forall\ f \in \mathbb{H}$ s.t. $\int_0^1 f(y)\,dy = 0$.

Thus, $i\hbar\psi - \zeta \perp f$ whenever $f \perp \{\text{constants}\}$. Thus,

$i\hbar\psi - \zeta$ is a constant function on $(0,1)$ and

$$i\hbar\psi = \zeta + \text{constant}.$$

Recalling $\zeta' = \eta = A_1^*\psi$ we conclude $\psi \in D(A_1^*)$ if and only if ψ has a derivative in $\mathbb{H}$ so $\psi \in D(A_3)$ and, moreover, $A_1\psi = i\hbar\psi'$ so $A_1^* = A_3$.

<u>Adjoint of A_2:</u> $\phi \in D(A_2) \Rightarrow \phi(0) = \phi(1)$. Also $\zeta(0) = 0$ by construction. So ⊕ reduces to $-\int_0^1 \overline{(i\hbar\psi)}\,\phi'\,dx = \zeta(1)\phi(1) - \int_0^1 \bar{\zeta}\phi'\,dx$ $\forall\, \phi \in D(A_2)$. Suppose this last identity holds true. By taking $\phi = \text{const} \neq 0$ we obtain $\zeta(1) = 0 = \zeta(0)$. Thus, the last identity is equivalent to $\int \overline{(i\hbar\psi - \zeta)}\, f\, dy$ $\forall\, f \in \mathbb{H}$ with $\int_0^1 f(y)\,dy = 0$. $\Leftrightarrow \psi' \in \mathbb{H}$.

Thus, we get $D(A_2^*) \subset D(A_3)$ and $i\hbar\psi = \zeta + \text{const}$. Then $\zeta(0) = \zeta(1) \Rightarrow \psi(0) = \psi(1)$ so $D(A_2^*) \subset D(A_2)$.
On the other hand, $\psi \in D(A_2) \Longrightarrow$ ⊕ holds with $\zeta = \psi - \psi(0)$ (s.t. $\zeta(0) = \zeta(1) = 0$.)

<u>Adjoint of A_3:</u> $A_3^* = A_1$

P is a <u>projection operator</u> if $P^2\psi = P\psi$ $\forall\, \psi \in \mathbb{H}$. An <u>orthogonal projection operator</u> P is symmetric $\Leftrightarrow$ (Nullspace of P) $N(P)$ $\perp R(P)$ (range of P) i.e. $\{\phi : P\phi = 0\} \perp \{P\psi : \psi \in \mathbb{H}\}$. is also a symmetric projection operator.

$A = \lim_{\sigma\to\sigma_0} A_\sigma$ means $A_\sigma \to A$ in the operator norm: $\lim_{\sigma\to\sigma_0} \|A_\sigma - A\| = 0$.

For bounded operators: $A = s\text{-}\lim A_\sigma$ means $\|A_\lambda\psi - A\psi\| \to 0$ $\forall\, \psi \in \mathbb{H}$.

If $A = \lim_{\sigma\to\sigma_0} A_\sigma$ then $A = s\text{-}\lim_{\sigma\to\sigma_0} A_\sigma$. (Converse is not true)

Existence of Dynamics: We say the dynamics exist for the Cauchy problem

$$(*)\quad \begin{cases} i\hbar\,\partial_t \psi = H\psi ; \\ \psi(0,x) = \psi_0(x) \in D(H) \end{cases}$$

iff $\exists !$ solution which conserves probability.

$$\boxed{\text{Theorem: Dynamics exist} \iff H \text{ is self-adjoint.}}$$

We prove $\Leftarrow$ following [GS; Ch 2]. (See [RS I] for $\Rightarrow$). For the purposes of our studies, the direction $\Leftarrow$ is the important statement.

Suppose $H : \mathbb{H} \to \mathbb{H}$ is a self-adjoint operator. Our task is to define the solution of $(*)$ and show the evolution conserves probability. We will carry this out in steps: (1) We define the exponential of a bounded operator. (2) We define e^{iA} for an unbounded self adjoint operator. (3) We define the solution $\psi(t) = e^{-iHt/\hbar}\psi_0$. (4) We show the propagator $U(t) = e^{-iHt/\hbar}$ is unitary on $L^2(\mathbb{R}^3)$. (5) We show $\psi(t)$ satisfies the PDE and takes on the initial value.

(1) Exponential of a bounded operator: $e^A := \sum_{n=0}^{\infty} \frac{A^n}{n!}$. This converges absolutely in the operator norm.

$$LS_V(\mathbb{R}^d) \begin{cases} i\hbar \frac{\partial}{\partial t}\psi = H\psi \quad ; \quad H\psi = \left[-\frac{\hbar^2}{2m}\Delta + V\right]\psi \\ \psi(0,x) = \psi_0(x) \end{cases}$$ V $\mathbb{R}$-valued, "nice"

Observe that H is symmetric: $\langle H\psi, \phi\rangle = \langle \psi, H\phi\rangle$ $\forall \psi, \phi \in D(H) \subset L^2(\mathbb{R}^d)$.

In fact, for "nice" V, H is even better than symmetric. H is self-adjoint.

Defn: The adjoint of an operator $A : \mathbb{H} \to \mathbb{H}$ is the operator A^* satisfying

$$\langle A^*\psi, \phi\rangle = \langle \psi, A\phi\rangle \qquad \forall \phi \in D(A)$$

$$\forall \psi \in D(A^*) = \{\psi \in \mathbb{H} : \langle \psi, A\phi\rangle \le C_\psi \|\phi\| \text{ for some } C_\psi \text{ (independent of } \phi \text{)} \ \forall \phi \in D(A)\}$$

Exercise Show that the definition of A^* defines a unique linear operator A^* on $D(A^*)$. (Hint: Riesz representation ...)

Defn: An operator A is self-adjoint if $A = A^*$.

- Self-adjoint = symmetric + $D(A) = D(A^*)$
- $\exists$ symmetric operators which are not self-adjoint,
- Not every symmetric operator can be uniquely extended to larger domain to become selfadjoint

Exercise Show that each of the following operators are symmetric.

- multiplication operator by $V(x)$ (if V $\mathbb{R}$-valued)
- Differentiation operator $P_j = -i\hbar\partial_j$
- Laplacian Δ
- Schrödinger operator $H = -\Delta + V$ (V $\mathbb{R}$-valued)
- Integral operator $Kf(x) = \int K(x,y) f(y)\,dy$ (if $K(x,y) = \overline{K(x,y)}$).

Lemma A bounded + symmetric $\Longrightarrow$ A self-adjoint

proof: A bounded $\Longrightarrow$ we may assume by extension $D(A) = \mathbb{H}$.
Since $|\langle \psi, A\phi \rangle| \leq \|\psi\| \, A \, \|\phi\|$ $\forall \psi, \phi$ we have
$D(A^*) = \mathbb{H}$ so $D(A) = D(A^*)$ and A self-adjoint

Exercise: Show $P_j = -i\hbar \partial_j$ and $T = -\frac{\hbar^2}{2m}\Delta$ are unbounded on $L^2(\mathbb{R}^d)$.

Theorem A self-adjoint.
$\forall z \in \mathbb{C}$ s.t. $\mathrm{Im}(z) \neq 0$, operator $A - z\mathbb{1}$ has bdd. inverse +

$$\circledast \qquad \|(A - z\mathbb{1})^{-1}\phi\| \leq |\mathrm{Im}(z)|^{-1}\|\phi\|.$$

proof: Suppose $\mathrm{Im}(z) \neq 0$. $\forall \psi \in D(A)$,

$$\|(A - z\mathbb{1})\psi\|^2 = \langle (A - z\mathbb{1})\psi, (A - z\mathbb{1})\psi \rangle$$
$$= \|A\psi\|^2 - 2\mathrm{Re}(z)\langle \psi, A\psi \rangle + \underbrace{|z|^2}_{|\mathrm{Re}(z)|^2 + (\mathrm{Im}(z))^2}\|\psi\|^2$$

$$\Longrightarrow \|(A - z\mathbb{1})\psi\|^2 \geq \|A\psi\|^2 - 2\mathrm{Re}(z)\|\psi\|\,\|A\psi\| + |z|^2\|\psi\|^2.$$
$$= (\|A\psi\| - |\mathrm{Re}(z)|\,\|\psi\|)^2 + |\mathrm{Im}(z)|^2\|\psi\|^2$$

$$\Longrightarrow \|(A - z\mathbb{1})\psi\| \geq |\mathrm{Im}(z)|\,\|\psi\|.$$

$\boxed{\#}$

This shows that $(A - z\mathbb{1})^{-1} : \mathrm{Ran}(A - z\mathbb{1}) \longrightarrow \mathbb{H}$ exists and satisfies $\circledast$.

Moreover, $\forall \phi \perp \mathrm{Ran}(A - z\mathbb{1})$ then $\langle \phi, (A - z\mathbb{1})\psi \rangle = 0$ $\forall \psi \in D(A)$.
Therefore, $0 = \langle \phi, (A - z\mathbb{1})\psi \rangle = \langle (A - \bar{z}\mathbb{1})\phi, \psi \rangle$ $\forall \psi \in D(A)$. Since $D(A)$ dense in $\mathbb{H}$, $(A - \bar{z}\mathbb{1})\phi = 0$. By $\boxed{\#}$
Thus, $\phi \in D(A^*) = D(A)$.
we conclude $\phi = 0$. Thus, $\mathrm{Ran}(A - z\mathbb{1})$ is dense in $\mathbb{H}$ so $(A - z\mathbb{1})^{-1}$ can be defined on $\mathbb{H}$ via extension, with $\circledast$ valid $\forall \phi \in \mathbb{H}$.

Exponential of a bounded operator $A : \mathbb{H} \to \mathbb{H}$.

<u>Lemma:</u> $A : \mathbb{H} \to \mathbb{H}$ bounded $\Longrightarrow e^A : \mathbb{H} \to \mathbb{H}$ exists & is bounded.

<u>proof:</u> $A : \mathbb{H} \to \mathbb{H}$ bounded means $\exists$ constant $\|A\|$

$$\|A\psi\|_{\mathbb{H}} \leq \|A\| \, \|\psi\|_{\mathbb{H}} \quad \forall \, \psi \in \mathbb{H}.$$

Form e^A with <u>formal power-series</u>.

$$e^A = \sum_{n=0}^{\infty} \frac{A^n}{n!}.$$

Note that the series converges absolutely so

$$\|e^A\| \leq \sum_{n=0}^{\infty} \frac{\|A^n\|}{n!} \leq \sum_{n=0}^{\infty} \frac{\|A\|^n}{n!} = e^{\|A\|} < \infty.$$

Thus, the limit exists and defines e^A uniquely.

<u>Exercise</u> Find e^{-iH} for 2×2 matrices $H = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $H = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

Imaginary Exponential of (unbounded) self-adjoint $A: D(A) \to \mathbb{H}$.

Lemma: A (unbounded) self-adjoint on $\mathbb{H} \implies e^{iA}: \mathbb{H} \to \mathbb{H}$ well-defined; bounded.

Rk: $A: D(A) \to \mathbb{H}$ for $D(A) \overset{\text{strict}}{\subsetneq} \mathbb{H}$ but $e^{iA}: \mathbb{H} \to \mathbb{H}$!

proof: (Introduce bounded approximators A_λ of A and study associated approximators e^{iA_λ} of e^{iA}.)

We define $A_\lambda = \frac{1}{2}\lambda^2 \left[(A+\lambda i)^{-1} + (A - i\lambda)^{-1} \right]$. We observe.

① A_λ well-defined, bounded $\forall \lambda > 0$.

② A_λ approximates A in sense that $A_\lambda \psi \to A\psi$ as $\lambda \to \infty$ $\forall \psi \in D(A)$.

① why? Because of lemmas above involving $(A - z\mathbb{1})^{-1}$.

② (intuition). Suppose A is a constant. Common denominators $\rightsquigarrow$

$$A_\lambda = \frac{1}{2}\lambda^2 \left[\frac{(A - i\lambda)}{A^2 + \lambda^2} + \frac{(A + i\lambda)}{A^2 + \lambda^2} \right] = \frac{\lambda^2}{2} \frac{2A}{A^2 + \lambda^2} \to A \text{ as } \lambda \to \infty.$$

② (formal)

$A_\lambda = B_\lambda A$ where $B_\lambda = \frac{1}{2}(i\lambda)\left[(A + i\lambda)^{-1} - (A - i\lambda)^{-1} \right]$ and

$$\mathbb{1} - B_\lambda = \frac{1}{2}\left[(A + i\lambda)^{-1} + (A - i\lambda)^{-1} \right] A.$$

Using $\|(A \pm i\lambda)^{-1}\| \le \frac{1}{\lambda}$ we find $\forall \phi \in D(A)$

$$\| (\mathbb{1} - B_\lambda)\phi \| \le \frac{1}{\lambda} \|A\phi\| \to 0 \quad \text{as} \quad \lambda \to \infty.$$

Since $D(A)$ dense and $\|B_\lambda\| \le 1$ we have $B_\lambda \phi \to \phi$ as $\lambda \to \infty$ $\forall \phi \in \mathbb{H}$! Taking $\phi = A\psi$ $\forall \psi \in D(A)$ we find $A_\lambda \psi \to A\psi$ as $\lambda \to \infty$.

Since A_λ bounded $\forall \lambda > 0$, we may define e^{iA_λ} by power series.

We show $\{ e^{iA_\lambda} : \lambda > 0 \}$ satisfies $\| (e^{iA_{\lambda'}} - e^{iA_\lambda}) \psi \| \to 0$ as $\lambda, \lambda' \to \infty$ $\forall \psi \in D(A)$. This proves $\{ e^{iA_\lambda} : \lambda > 0 \}$ is a Cauchy family.

This will permit us to define $e^{iA} : \mathbb{H} \to \mathbb{H}$.

By FTOC:

$$e^{iA_{\lambda'}} - e^{iA_\lambda} = \int_0^1 \frac{\partial}{\partial s} \left(e^{isA_{\lambda'}} e^{i(1-s)A_\lambda} \right) ds .$$

Since A_λ symmetric and bounded, A_λ is self-adjoint.

Problem: Using power series representation, show that if A is a bounded operator, then

①. $\frac{\partial}{\partial s} e^{isA} = iA e^{isA} = e^{isA} iA$. (commutativity ?)

② If A is self-adjoint then e^{iA} is an isometry:

$$\| e^{iA} \psi \| = \| \psi \| .$$

Using the steps from the problem, we find using FTOC formula that

$$\| (e^{iA_{\lambda'}} - e^{iA_\lambda}) \psi \| = \left\| \int_0^1 e^{isA_{\lambda'}} e^{i(1-s)A_\lambda} \left[i(A_{\lambda'} - A_\lambda) \right] \psi \, ds \right\|$$

$$\leq \int_0^1 \| e^{isA_{\lambda'}} e^{i(1-s)A_\lambda} i(A_{\lambda'} - A_\lambda) \psi \| \, ds$$

$$= \int_0^1 \| (A_\lambda - A_{\lambda'}) \psi \| \, ds = \| (A_{\lambda'} - A_\lambda) \psi \| \to 0 .$$

Thus, $\forall \psi \in \mathcal{D}(A)$ the vectors $e^{iA_\lambda} \psi$ converge to some element of $\mathbb{H}$ as $\lambda \to \infty$.

Moreover, we call this element $e^{iA} \psi$ and observe $\| e^{iA} \psi \| \leq \| \psi \|$ $\forall \psi \in D(A)$.

By density, e^{iA} extends to all of $\mathbb{H}$, so $e^{iA} : \mathbb{H} \to \mathbb{H}$ is well-defined, bounded.

Unitary Operators

Definition An operator U is called unitary if $UU^* = U^*U = 1$.

Unitary operators are isometries:

$$\langle U\psi, U\phi\rangle = \langle\psi, U^*U\phi\rangle = \langle\psi,\phi\rangle. \implies \|U\psi\| = \|\psi\|.$$

Thus, unitary operators are bounded operators with operator norm 1.

Unitary operators are invertible with inverse equal to its adjoint

Theorem: A self-adjoint $\implies e^{iA}$ unitary.

Exercise: Using power series representation of e^{iA}, prove theorem for bounded A.

Assuming the exercise, we prove theorem for unbounded A. By definition, we have $e^{iA}\psi = \lim_{\lambda\to\infty} e^{iA_\lambda}\psi$ so

$$\langle e^{iA}\psi, e^{iA}\phi\rangle = \lim_{\lambda\to\infty}\langle e^{iA_\lambda}\psi, e^{iA_\lambda}\phi\rangle = \langle\psi,\phi\rangle$$

$\implies (e^{iA})^* e^{iA} = 1$. Similarly, $(e^{iA})^* = e^{-iA}$. Revisiting preceding argument with e^{iA} replaced by e^{-iA} gives

$e^{iA}(e^{iA})^* = 1$ so e^{iA} is unitary.

H self-adjoint $\Longrightarrow$ existence of dynamics

proof: H self-adjoint $\Longrightarrow$ $U(t) = e^{-iHt/\hbar}$ exists and is unitary $\forall t \in \mathbb{R}$.

(Note that $Ht/\hbar$ self-adjoint)

Thus, $U(t)\psi_0 = \psi(t)$ satisfies $\|\psi(t)\| = \|\psi_0\|$.

This implies that $\psi_0 \longmapsto \psi(t) = U(t)\psi_0$ conserves probability.

Next we show $\psi(t)$ satisfies the PDE.

Recall $e^{-iHt/\hbar}\psi_0 = \lim_{\lambda\to\infty} e^{-iH_\lambda t/\hbar}\psi_0$ where

$H_\lambda = \frac{1}{2}\lambda^2\left[(H+i\lambda)^{-1} + (H-i\lambda)^{-1}\right]$ are bounded operators. We

have $\frac{\partial}{\partial t} e^{-iH_\lambda t/\hbar}\psi_0 = -\frac{i}{\hbar} H_\lambda e^{-iH_\lambda t/\hbar}\psi_0$.

Thus, (with some justifiable formal steps) we have

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}\langle \phi, e^{-iHt/\hbar}\psi_0\rangle &= i\hbar \frac{\partial}{\partial t}\lim_{\lambda\to\infty}\langle \phi, e^{-iH_\lambda t/\hbar}\psi_0\rangle \\
&= i\hbar \lim_{\lambda\to\infty}\langle \phi, \frac{\partial}{\partial t} e^{-iH_\lambda t/\hbar}\psi_0\rangle \\
&= \lim_{\lambda\to\infty}\langle \phi, H_\lambda e^{-iH_\lambda t/\hbar}\psi_0\rangle \\
&= \lim_{\lambda\to\infty}\langle H_\lambda\phi, e^{-iH_\lambda t/\hbar}\psi_0\rangle \\
&= \langle H\phi, e^{-iHt/\hbar}\psi_0\rangle .
\end{aligned}
$$

Therefore, $i\hbar \frac{\partial}{\partial t} e^{-iHt/\hbar}\psi_0 = H e^{-iHt/\hbar}\psi_0$ so

$\psi(t) = e^{-iHt/\hbar}\psi_0$ satisfies the PDE!

Certainly $U(0) = 1$. Moreover, $\forall\ \psi_0 \in D(H)$,

$$U(t)\psi_0 - \psi_0 = \frac{i}{\hbar}\int_0^t U(s)\, H\psi_0 \, ds \longrightarrow 0 \text{ as } t \to 0$$

Thus, the initial condition also holds true.

Note that the solution operator is uniquely defined. Indeed suppose we had 2 solutions $\psi_1(t)$ and $\psi_2(t)$ emerging from the given initial data ψ_0. Their difference $\tilde{\psi}(t) = \psi_1(t) - \psi_2(t)$ solves same PDE with initial data $\tilde{\psi}(0) = \psi_0 - \psi_0 = 0$. Thus, by probability conservation, $\|\tilde{\psi}(t)\| = \|\tilde{\psi}(0)\| = 0\ \forall\ t$ so $\tilde{\psi} \equiv 0$. This completes proof of our theorem. ∎

The operator family $U(t) = e^{-iHt/\hbar}$ is called the *propagator* or evolution operator. This operator has a group property

$$U(t)\,U(s) = U(t+s) \quad \forall\ t, s \in \mathbb{R}.$$

Exercise: Show that $e^{-iH_0 t/\hbar}$ has the group property. (Use power series representation ...)

Assuming the exercise, we proceed as before to justify the group property for $U(t)$: $\forall\ \phi, \psi \in \mathbb{H}$

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

$$= \lim_{\lambda\to\infty} \langle e^{iH_\lambda t/\hbar}\psi, e^{-iH_\lambda s/\hbar}\phi \rangle$$

$$= \lim_{\lambda\to\infty} \langle \psi, e^{-iH_\lambda (s+t)/\hbar}\phi \rangle$$

$$= \langle \psi, U(t+s)\phi \rangle.$$

Thus, $\quad U(t)U(s) = U(t+s).$

Observables; Fourier Transform QM Course 2008 (lecture #5)

[GS: 25–26]

Observables: These are the quantities that can be measured experimentally.

At time t, the state or configuration of a physical system, such as a particle, is described by a wave function $\psi(t, \underline{x})$. The interpretation is that the probability of finding the particle in some subset $\Omega \subset \mathbb{R}^d$ is given by $\int_{\mathbb{R}^d} |\psi(t,\underline{x})|^2 \, d\underline{x}$. We can therefore formulate probabilistic answers to natural questions. Where is the particle located? Best guess: $\int_{\mathbb{R}^d} \underline{x} \, |\psi(t,\underline{x})|^2 d\underline{x}$. We can also address other issues but let's linger here and consider the coordinate multiplication operator $x_j : \psi(t, \cdot) \longmapsto (\cdot)_j \, \psi(t, \cdot)$ in more detail.

The mean value of the jth coordinate component of $\underline{x}$ in the state $\psi(t,\cdot)$ is $\langle \psi, x_j \psi \rangle$. How does this mean value behave with time? The answer depends upon how ψ behaves with time, which is governed by Schrödinger's equation. We calculate: (using $i\hbar \frac{\partial}{\partial t}\psi = H\psi, \ldots$)

$$\frac{d}{dt} \langle \psi, x_j \psi \rangle = \langle \dot{\psi}, x_j \psi \rangle + \langle \psi, x_j \dot{\psi} \rangle$$

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

$$= \left\langle \psi, \frac{i}{\hbar} H x_j \psi \right\rangle - \left\langle \psi, \frac{i}{\hbar} x_j H \psi \right\rangle$$

$$= \left\langle \psi, \frac{i}{\hbar} [H, x_j] \psi \right\rangle .$$

We have introduced the commutator $[A, B] = AB - BA$. Summarizing, we have found

$$\frac{d}{dt} \langle \psi, x_j \psi \rangle = \left\langle \psi, \frac{i}{\hbar} [H, x_j] \psi \right\rangle .$$

We specialize to the case where $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$. A simple calculation shows that

$$\frac{i}{\hbar}[H, x_j] = -\frac{i\hbar}{m}\partial_j .$$

We carry out this calculation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V,\ x_j\right]\psi = -\frac{\hbar^2}{2m}\Delta(x_j\psi) + x_j\frac{\hbar^2}{2m}\Delta\psi = \frac{\hbar^2}{2m}\left[x_j\Delta\psi - \Delta(x_j\psi)\right]$$

$$\Delta(x_j\psi) = \partial_k\partial_k(x_j\psi) = \partial_k(\delta_{jk}\psi + x_j\psi_k) = \delta_{jk}\psi_k + \delta_{jk}\psi_k + x_j\Delta\psi .$$

$$\frac{i}{\hbar}[H, x_j] = \frac{i}{\hbar}\left[2\frac{\hbar^2}{2m}\partial_j\psi\right] = \frac{i\hbar}{m}\partial_j\psi . \quad \checkmark$$

For an operator A, the expression $\langle\psi, A\psi\rangle$ represents the mean value of A in the state ψ. Let us denote $\langle\psi, A\psi\rangle = \langle A\rangle_\psi$.

We can then write, using the calculations above,

$$m\frac{d}{dt}\langle x_j\rangle_\psi = \langle -i\hbar\partial_j\rangle_\psi .$$

This is a quantum analog of $m\underline{\dot{x}} = \underline{p}$ so we define $p_j = -i\hbar\partial_j$.

The operator $\underline{p} = -i\hbar\underline{\nabla}$ is called the <u>momentum operator</u>.

<u>Definition</u> An <u>observable</u> is any self-adjoint operator on the state space $L^2(\mathbb{R}^d)$.

<u>Examples:</u> x_j, p_j, Schrödinger operator H, angular momentum operator $L_j = (\underline{x} \times \underline{p})_j$. Note that $H = \frac{1}{2m}|\underline{p}|^2 + V$.

Exercise 5.1 For any observable A, check that

$$\frac{d}{dt}\langle A\rangle_\psi = \langle \psi, \frac{i}{\hbar}[H, A]\psi\rangle.$$

Apply this calculation to establish $\frac{d}{dt}\langle P_j\rangle_\psi = \langle -\partial_j V\rangle_\psi$, provided that ψ satisfies $LS_V(\mathbb{R}^d)$. Compare this with Newton's equation.

Since $[H, H] = 0$, we have $\frac{d}{dt}\langle H\rangle_\psi = 0$. This the mean value (quantum analog) of energy conservation.

The Fourier Transform:

The Fourier transform provides a representation of functions in a basis of eigenfunctions of differentiation. As a result, it is fantastically useful and appears ubiquitously in mathematics, science and engineering.

We follow some of the discussion in [Lieb-Loss "Analysis"; Ch. 5].

Fourier Transform on L^1

$\forall \; f \in L^1(\mathbb{R}^n)$ we define

$$\hat{f}(\underline{k}) = \int_{\mathbb{R}^n} e^{-2\pi i \underline{k}\cdot\underline{x}} f(\underline{x})\, dx$$

where $\quad \underline{k}\cdot\underline{x} = \sum_{i=1}^{n} k_i x_i .$

Note that the integral makes sense for $f \in L^1(\mathbb{R}^n)$. Indeed $\|\hat{f}\|_{L^\infty} \le \|f\|_{L^1}$.

<u>Exercise 5.2</u> (Algebraic properties of the Fourier transform) Prove the following (easy) facts about the Fourier transform:

- The map $f \longmapsto \hat{f}$ is linear in f.
- If $(\tau_h f)(x) = f(x-h)$ then $(\tau_h f)^\wedge(k) = e^{-2\pi i \underline{k}\cdot\underline{h}} \hat{f}(k)$, $h \in \mathbb{R}^n$.
- If $(\delta_\lambda f)(x) = f\left(\frac{x}{\lambda}\right)$ then $(\delta_\lambda f)^\wedge(k) = \lambda^n \hat{f}(\lambda k)$, $\lambda > 0$.

<u>Exercise 5.3</u> Suppose $f \in L^1(\mathbb{R}^n)$. Prove that $\hat{f}$ is continuous and, moreover, that $\hat{f}(k) \longrightarrow 0$ as $|k| \to \infty$. (Hint: This is called the Riemann-Lebesgue Lemma.)

<u>Exercise 5.4</u> Suppose ψ is a C^∞ function supported on $[-1,1] \subset \mathbb{R}$. Consider the integral $\quad I_\lambda = \int_{\mathbb{R}} e^{i\lambda x^3} \psi(x)\, dx$. Certainly, $|I_\lambda| \le \|\psi\|_{L^1}$. Find the behavior of I_λ as $\lambda \longrightarrow \infty$.

Fourier Transform of a Gaussian

For $\lambda > 0$ define $g_\lambda(x) = e^{-\pi\lambda|x|^2}$ for $x \in \mathbb{R}^n$.

Then $$\hat{g}_\lambda(k) = \lambda^{-\frac{n}{2}} e^{-\pi|k|^2/\lambda}.$$

Exercise 5.5 Prove the formula for $\hat{g}_\lambda$.

Fourier Transform on L^2

Plancherel's Theorem. If $f \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ then $\hat{f} \in L^2(\mathbb{R}^n)$ and

$$\|\hat{f}\|_{L^2} = \|f\|_{L^2}.$$

The map $f \mapsto \hat{f}$ has a unique extension to a continuous linear map from $L^2(\mathbb{R}^n) \longrightarrow L^2(\mathbb{R}^n)$ which is an isometry. The extended map is still denoted $f \mapsto \hat{f}$.

If $f, g \in L^2(\mathbb{R}^n)$ then Parseval's formula holds:

$$\langle f, g\rangle = \int_{\mathbb{R}^n} \bar{f}(x) g(x)\, dx = \int_{\mathbb{R}^n} \overline{\hat{f}(k)}\, \hat{g}(k)\, dk = \langle \hat{f}, \hat{g}\rangle.$$

proof: For $f \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ we have $\hat{f}(\cdot)$ bounded. Therefore,

(*) $\int_{\mathbb{R}^n} |\hat{f}(k)|^2 e^{-\varepsilon\pi|k|^2}\, dk$ is defined for all $\varepsilon > 0$. Since $f \in L^1(\mathbb{R}^n)$, the function $\bar{f}(x) f(y) e^{-\varepsilon\pi|k|^2} \in L^1(\mathbb{R}^n_x \times \mathbb{R}^n_y \times \mathbb{R}^n_k)$.

We can reexpress this relation. Substitute definition of $\hat{f}(k)$ and rewrite. By Fubini's theorem and the Fourier transform property of Gaussians,

$$\int_{\mathbb{R}^{3n}} \bar{f}(x) f(y) e^{2\pi i \underline{k}\cdot(\underline{x}-\underline{y})} e^{-\varepsilon\pi|k|^2} dx\,dy\,dk = \int_{\mathbb{R}^{2n}} \varepsilon^{-\frac{n}{2}}\left(e^{-\frac{\pi|x-y|^2}{\varepsilon}}\right) \bar{f}(x) f(y)\,dx\,dy.$$

By approximation, we know that

$$\varepsilon^{-n/2} \int e^{-\frac{\pi(x-y)^2}{\varepsilon}} f(y)\,dy \longrightarrow f(x), \quad \text{in } L^2(\mathbb{R}^n) \quad \text{as } \varepsilon \to 0.$$

Therefore, we have that $\int |\hat{f}(k)|^2 e^{-\varepsilon\pi|k|^2} dk \longrightarrow \int |f(x)|^2 dx$ as $\varepsilon \to 0$. This proves (*) is uniformly bounded in $\varepsilon > 0$ and the monotone convergence theorem shows that $\hat{f} \in L^2(\mathbb{R}^n)$, with $\|\hat{f}\|_{L^2} = \|f\|_{L^2}$.

Now, let $f \in L^2(\mathbb{R}^n)$ but not in $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$. Since $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ $\exists$ $(f^j) \subset L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ such that $\|f - f^j\|_{L^2} \to 0$ as $j \to \infty$. We know that $\|\hat{f}^j - \hat{f}^m\|_{L^2} = \|f^j - f^m\|_{L^2}$ and therefore $\hat{f}^j$ is Cauchy in $L^2(\mathbb{R}^n)$. We call the limit $\hat{f}$ since it is clear that $\hat{f}$ does not depend upon the choice of the subsequence.

The parseval relation follows from the isometry property and some algebra.

<u>Remark</u>: Given $f \in L^2$, we can compute its Fourier transform $\hat{f} \in L^2$. The way we do so is to consider <u>any</u> approximating sequence $f^j \in L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$ such that $\|f^j - f\|_{L^2} \to 0$ as $j \to \infty$. We always find a unique limit of the sequence $\hat{f^j}$ which does not depend upon the sequence f^j, only upon the function $f \in L^2$!

The map $f \longmapsto \hat{f}$ is not just an isometry on L^2. In fact, it is a unitary transformation, an invertible isometry.

<u>Inversion Formula</u>

For $f \in L^2(\mathbb{R}^n)$, we define $f^{\vee}(x) = \hat{f}(-x)$ (which amounts to replacing i by $-i$ in the definition of $\hat{f}$). Then, we have

$$f = (\hat{f})^{\vee}.$$

<u>proof</u>: $\forall\, f \in L^2(\mathbb{R}^n)$, we have

$$\circledast \quad \int_{\mathbb{R}^n} \hat{g}_\lambda(y-x)\, f(y)\, dy = \int g_\lambda(k)\, \hat{f}(k)\, e^{2\pi i \underline{k} \cdot \underline{x}}\, dk .$$

This follows from Plancherel's theorem and an approximation $L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n) \ni f_j \to f \in L^2$.

Next, we take $\lambda \to 0$. Then the left side of $\circledast$ tends to $f(x)$ in $L^2(\mathbb{R}^n)$. On the right side, as $\lambda \to 0$, we have $g_\lambda \hat{f} \longrightarrow \hat{f}$ in $L^2(\mathbb{R}^n)$ (by dominated convergence theorem) so we find that $(g_\lambda \hat{f})^{\vee} \longrightarrow (\hat{f})^{\vee}$ in $L^2(\mathbb{R}^n)$. Equating the $\lambda \to 0$ limits of both sides of $\circledast$ proves the inversion formula.

Fourier Transform in $L^p(\mathbb{R}^n)$:

We know:

$$f \in L^1(\mathbb{R}^n) \implies \hat{f} \in L^\infty(\mathbb{R}^n) \quad \text{with} \quad \|\hat{f}\|_{L^\infty} \le \|f\|_{L^1}.$$

$$f \in L^2(\mathbb{R}^n) \implies \hat{f} \in L^2(\mathbb{R}^n) \quad \text{with} \quad \|\hat{f}\|_{L^2} = \|f\|_{L^2}.$$

Note: Not every $L^\infty(\mathbb{R}^n)$ function is the Fourier transform of some $L^1(\mathbb{R}^n)$-function. So, the Fourier transform is *not* invertible on $L^1(\mathbb{R}^n)$.

Exercise 5.6 Suppose $1 < p < 2$. Consider the inequality

$$\|\hat{f}\|_{L^q(\mathbb{R}^n)} \le C \, \|f\|_{L^p(\mathbb{R}^n)}.$$

Using the Fourier transform property of Gaussians and the scaling property, prove that this inequality can only hold for a particular choice of q depending upon p.

Hausdorff - Young Theorem

If $1 < p < 2$ and $f \in L^p(\mathbb{R}^n) \cap L^1(\mathbb{R}^n)$ then, with $\frac{1}{p} + \frac{1}{p'} = 1$,

$$\|\hat{f}\|_{L^{p'}} \leq C_p^n \|f\|_{L^p}$$

for some constant C_p^n depending only upon n and p.

Convolutions

Let $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$ and let $1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}$.

Suppose $1 \leq p, q, r \leq 2$. Then

$$(f * g)^\wedge(k) = \hat{f}(k)\,\hat{g}(k).$$

Here $(f*g)(x) = \int_{\mathbb{R}^n} f(x-y)\,g(y)\,dy$.

Fourier Transform and Convolutions; ~~Applications to PDE + QM~~ (lecture #6)

QM Course 2008

[Lieb + Loss; Ch. 4 + Ch. 5], [Stein-Weiss]

Given $f, g : \mathbb{R}^n \to \mathbb{C}$, we define their convolution to be the function

$$(f * g)(x) = \int_{\mathbb{R}^n} f(x-y)\, g(y)\, dy.$$

We have $f*g = g*f$ by a change of variables. Does $f*g$ make sense?

If $f \in L^p(\mathbb{R}^n)$ and $g \in L^{p'}(\mathbb{R}^n)$, certainly $f*g \in L^\infty(\mathbb{R}^n)$ by Hölder's inequality.

Fact: If $f \in L^p(\mathbb{R}^n)$, $1 \le p \le \infty$ and $g \in L^1(\mathbb{R}^n)$ then $f*g$ is well-defined and $f*g \in L^p(\mathbb{R}^n)$ with

$$\|f*g\|_{L^p(\mathbb{R}^n)} \le \|f\|_{L^p(\mathbb{R}^n)} \|g\|_{L^1(\mathbb{R}^n)}.$$

proof:

$$|f*g(x)| \le \int_{\mathbb{R}^n} |f(x-y)|\,|g(y)|\, dy.$$

$$\left(\int |f*g(x)|^p dx\right)^{\frac{1}{p}} \le \left(\int_{\mathbb{R}^n} \left|\int_{\mathbb{R}^n} |f(x-y)|\,|g(y)|\, dy\right|^p\right)^{\frac{1}{p}}$$

Minkowski's integral inequality.

$$\le \left[\int_{\mathbb{R}^n}\left(\int_{\mathbb{R}^n} |f(x-y)|^p |g(y)|^p dx\right)^{\frac{1}{p}} dy\right].$$

$$= \int_{\mathbb{R}^n} |g(y)| \left(\int_{\mathbb{R}^n} |f(x-y)|^p dx\right)^{\frac{1}{p}}$$

$$= \|g\|_{L^1} \|f\|_{L^p}. \quad \blacksquare$$

> Rk. We used this before to build smooth approximators to $f \in L^p$.

More generally, we have Young's inequality for convolutions.

<u>Theorem</u> (Young's Inequality for Convolutions)

Let $p, q, r \geq 1$. Let $\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 2$.

Let $f \in L^p(\mathbb{R}^n)$, $g \in L^q(\mathbb{R}^n)$, $h \in L^r(\mathbb{R}^n)$.

Then

$$\circledast \quad \left| \int_{\mathbb{R}^n} f(x) \, (g * h)(x) \, dx \right| = \left| \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x) \, g(x-y) \, h(y) \, dx \, dy \right|$$

$$\leq C \, \|f\|_p \, \|g\|_q \, \|h\|_r .$$

<u>proof</u> Introduce, p', q', r', the Hölder dual exponents such that $\frac{1}{p} + \frac{1}{p'} = 1$, etc. Note that $(1 - \frac{1}{p'}) + (1 - \frac{1}{q'}) + (1 - \frac{1}{r'}) = 2$

so $\frac{1}{p'} + \frac{1}{q'} + \frac{1}{r'} = 1$. We now make a clever multiplicative decomposition of the integrand:

$$\alpha(x,y) = |f(x)|^{\frac{p}{r'}} \, |g(x-y)|^{\frac{q}{r'}}$$

(Assume, $f, g, h \geq 0$.)

$$\beta(x,y) = |g(x-y)|^{\frac{q}{p'}} \, |h(y)|^{\frac{r}{p'}}$$

$$\gamma(x,y) = |f(x)|^{\frac{p}{q'}} \, |h(y)|^{\frac{r}{q'}} .$$

Note that

$$\alpha(x,y) \, \beta(x,y) \, \gamma(x,y) = f(x)^{p\left(\frac{1}{r'} + \frac{1}{q'}\right)} \, g(x-y)^{q\left(\frac{1}{p'} + \frac{1}{r'}\right)} \, h(y)^{r\left(\frac{1}{p'} + \frac{1}{q'}\right)} .$$

Since $\frac{1}{r'} + \frac{1}{q'} = 1 - \frac{1}{p'} = \frac{1}{p}$, etc. we find

$$\alpha(x,y) \, \beta(x,y) \, \gamma(x,y) = f(x) \, g(x-y) \, h(y) .$$

By Hölder's inequality,

$$\circledast \leq \|\alpha\|_{p'} \, \|\beta\|_{q'} \, \|\gamma\|_{r'} .$$

Look at

$$\|\alpha\|_{r'} = \left(\int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x)^p \, g(x-y)^q \, dx \, dy \right)^{\frac{1}{r'}} = \|f\|_p^{p/r'} \, \|g\|_q^{q/r'} .$$

$$\|\beta\|_{p'} = \|g\|_q^{\frac{q}{p'}} \, \|h\|_r^{\frac{r}{p'}}$$

$$\|\gamma\|_{q'} = \|f\|_p^{\frac{p}{q'}} \, \|h\|_r^{\frac{r}{q'}} .$$

$$\|\alpha\|_{r'} \, \|\beta\|_{p'} \, \|\gamma\|_{q'} = \|f\|_p^{p\left(\frac{1}{r'} + \frac{1}{q'}\right)} \, \|g\|_q^{q\left(\frac{1}{r'} + \frac{1}{p'}\right)} \, \|h\|_r^{r\left(\frac{1}{p'} + \frac{1}{q'}\right)} .$$

But $\frac{1}{r'} + \frac{1}{q'} = 1 - \frac{1}{p'} = \frac{1}{p}$, etc.

Therefore,

$$\circledast \leq C \, \|f\|_p \, \|g\|_q \, \|h\|_r .$$

<u>Corollary</u> (Rewritten Young's Inequality).

$$\|g * h\|_{L^{p'}} \leq \|g\|_{L^q} \, \|h\|_{L^r}$$

provided $1 \leq p', q, r$ satisfy $\frac{1}{p'} = \frac{1}{q} + \frac{1}{r} - 1$.

<u>proof</u>:

$$\|g * h\|_{L^{p'}} = \sup_{\substack{f \in L^p \\ \|f\|_{L^p} \leq 1}} \int f(x) \, (g * h)(x) \, dx .$$

Note: $p' = 1$ requires $q = r = 1$ and the <u>Fact</u>: above applies.

Fourier Transform and convolutions

$$(f*g)^\wedge(k) = \int_{\mathbb{R}^n} e^{-2\pi i\, \underline{k}\cdot\underline{x}} (f*g)(x)\, dx$$

$$= \int_{\mathbb{R}^n} e^{-2\pi i\, \underline{x}\cdot\underline{k}} \int f(x-y)\, g(y)\, dy \quad dx$$

$$= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{-2\pi i\, ((\underline{x}-\underline{y})\cdot k)} f(x-y) \quad e^{-2\pi i\, \underline{y}\cdot\underline{k}} g(y)\, dx\, dy$$

$$= \int_{\mathbb{R}^n}\int_{\mathbb{R}^n} e^{-2\pi i\, (\underline{x}-\underline{y})\cdot\underline{k}} f(x-y)\, dx \quad e^{-2\pi i\, \underline{y}\cdot\underline{k}} g(y)\, dy$$

$$z = x - y$$
$$dz = dx$$

$$= \int_{\mathbb{R}^n} e^{-2\pi i\, \underline{z}\cdot\underline{k}} f(z)\, dz \quad \int_{\mathbb{R}^n} e^{-2\pi i\, \underline{y}\cdot\underline{k}} g(y)\, dy$$

$$= \hat{f}(k)\ \hat{g}(k).$$

The formal manipulations above, involving Fubini and change of variable, can be justified using the facts we know, namely Hausdorff-Young inequality and Young's inequality for convolutions.

Thus, integral operators given by convolution are equivalently described as multiplication operators on the Fourier transform side:

$$(T_k f)(x) = \int k(x-y)\, f(y)\, dy = (k * f)(x).$$

$$(T_k f)^\wedge(\xi) = \hat{k}(\xi)\, \hat{f}(\xi).$$

$$(T_k f)(x) = (\hat{k}\cdot\hat{f})^\vee(x).$$

Fourier Transform of certain homogeneous functions

Fourier Transform of $|x|^{\alpha-n}$

Let $f \in C_0^\infty(\mathbb{R}^n)$ and let $0 < \alpha < n$. Then, with $c_\alpha = \pi^{-\alpha/2}\,\Gamma(\alpha/2)$

$$c_\alpha \left(|k|^{-\alpha}\, \hat{f}(k) \right)^{\vee}(x) \;=\; c_{n-\alpha} \int_{\mathbb{R}^n} |x-y|^{\alpha-n} f(y)\, dy .$$

Since $f \in C_0^\infty(\mathbb{R}^n)$, $\hat{f}$ is very nice, (in fact it is an entire function of exponential type). As $|k| \to \infty$, $\hat{f}$ and all its derivatives decay faster than $|k|^{-r}$ for any $r > 0$. Therefore,

$$|k|^{-\alpha}\, \hat{f}(k) \in L^1(\mathbb{R}^n)$$

and we know it has a Fourier transform.

<u>proof</u>: We start from a basic formula:

$$c_\alpha |k|^{-\alpha} = \int_0^\infty e^{-\pi |k|^2 \lambda}\, \lambda^{\frac{\alpha}{2}-1}\, d\lambda .$$

Why? Recall that $\Gamma(z) = \int_0^\infty t^{z-1} e^{-t}\, dt$.

$$\int_0^\infty e^{-\pi|k|^2\lambda}\, \lambda^{\frac{\alpha}{2}-1}\, d\lambda \;=\; \int_0^\infty e^{-t} \left(\frac{t}{\pi|k|^2}\right)^{\frac{\alpha}{2}-1} \frac{1}{\pi|k|^2}\, dt$$

$t = \pi|k|^2\lambda$

$dt = \pi|k|^2 d\lambda$

$$= \int_0^\infty e^{-t}\, t^{\frac{\alpha}{2}-1} \cdot (\pi|k|^2)^{1-\frac{\alpha}{2}-1}\, dt$$

$$= (\pi|k|^2)^{-\frac{\alpha}{2}} \int_0^\infty e^{-t}\, t^{\frac{\alpha}{2}-1}\, dt$$

$$= \pi^{-\frac{\alpha}{2}}\, \Gamma\!\left(\tfrac{\alpha}{2}\right) |k|^{-\alpha} \quad \checkmark .$$

Since $|k|^{-\alpha} \hat{f}(k)$ is integrable, we have by Fubini's theorem

$$c_\alpha \left(|k|^{-\alpha} \hat{f}(k)\right)^{\vee}(x) = \int_{\mathbb{R}^n} e^{2\pi i \underline{k} \cdot \underline{x}} \left\{ \int_0^\infty e^{-\pi |k|^2 \lambda} \lambda^{\frac{\alpha}{2}-1} \, d\lambda \right\} \hat{f}(k) \, dk$$

$$= \int_0^\infty \left\{ \int_{\mathbb{R}^n} e^{2\pi i \underline{k} \cdot \underline{x}} \left[e^{-\pi |k|^2 \lambda} \hat{f}(k) \right] dk \right\} \lambda^{\frac{\alpha}{2}-1} \, d\lambda$$

F.T. of Gaussian + Convolution property

$$= \int_0^\infty \lambda^{-\frac{n}{2}} \lambda^{\frac{\alpha}{2}-1} \left\{ \int_{\mathbb{R}^n} e^{-\frac{\pi |x-y|^2}{\lambda}} f(y) \, dy \right\} d\lambda$$

$$= \int_{\mathbb{R}^n} \left[\int_0^\infty \lambda^{\frac{\alpha-n}{2}-1} e^{\frac{-\pi |x-y|^2}{\lambda}} \, d\lambda \right] f(y) \, dy$$

$$[\quad] = \int_0^\infty \left(\frac{1}{\mu}\right)^{\frac{\alpha-n}{2}-1} e^{-\pi |x-y|^2 \mu} \frac{1}{\mu^2} \, d\mu$$

$\mu = \frac{1}{\lambda}$

$d\mu = -\frac{1}{\lambda^2} d\lambda$

$$= \int_0^\infty \mu^{\frac{n-\alpha}{2}+1-2} e^{-\pi |x-y|^2 \mu} \, d\mu$$

$$= c_{n-\alpha} |x|^{\alpha-n}.$$

Lecture # 7   <u>Diffusion Equation / Free Schrödinger Equation</u>   28 october 2008   7.1

APM 421 ; QM

We will sometimes follow [Strauss; Intro PDE §2.4, §9.4].

<u>Diffusion on the line</u>

Initial Value problem for the diffusion/heat equation on the line.

$$(*) \quad \begin{cases} \partial_t u = \underbrace{K}_{\text{diffusion coefficient}} \partial_x^2 u & -\infty < x < +\infty, \quad 0 < t < \infty \\ u(0,x) = \underbrace{\phi(x)}_{\text{initial data}}. \end{cases}$$

We'd like to predict $u(t,x)$ for $t > 0$ from knowledge of initial data ϕ.

Before solving the problem for <u>general</u> ϕ, we will first find the solution for <u>special</u> ϕ and will build the general solution using the special ones.

<u>Basic Invariance Properties</u>

(translation) $u(t,x)$ Ⓢ $(*)$ $\iff$ $u(t, x-y)$ Ⓢ $(*)$.

(derivative) u Ⓢ $(*)$ $\implies$ $\partial_x u$, $\partial_t u$ both solve $(*)$, etc.

(superposition) u, v Ⓢ $(*)$ $\implies$ $au + bv$ Ⓢ $(*)$

$\{u_n\}_{n>0}$ Ⓢ $(*)$ $\implies$ $\int_0^\infty f_n u_n \, dn$ Ⓢ $(*)$.

(dilation) u Ⓢ $(*)$ $\implies$ $u_a(t,x) = u(\sqrt{a}\,x, at)$ $\forall a > 0$.

We seek a solution emerging from heaviside initial data.

<u>Heaviside Initial Data</u>

$$Q(0,x) = \begin{cases} 1 & x > 0, \\ 0 & x < 0. \end{cases}$$

<u>Note</u>: $Q_a = Q$. This data in <u>invariant</u> under dilation symmetry.

<u>Task</u>: Solve $(*)$ with $u(0,x) = Q(x)$. Denote solution $Q(t,x)$.

Step 1: Since $Q(0,x)$ is dilation invariant, we guess that $Q(t,x)$ is also dilation invariant. How can we express that assumption mathematically? We look for

$$(\text{self-similar}) \quad Q(t,x) = g(p) \quad \text{with} \quad p = \frac{x}{\sqrt{4Kt}}.$$

Note: $x \to \sqrt{a}\,x, \; t \mapsto at, \; p \longmapsto \dfrac{\sqrt{a}\,x}{\sqrt{4K(at)}} = \dfrac{x}{\sqrt{4Kt}} = p.$

Step 2: Using the (self similar) form, we convert the diffusion equation ⊛ for Q into an ODE for g.

$$Q_t = \frac{dg}{dp}\frac{\partial p}{\partial t} = -\frac{1}{2t}\frac{x}{\sqrt{4Kt}}\, g'(p).$$

$$Q_x = \frac{dg}{dp}\frac{\partial p}{\partial x} = \frac{1}{\sqrt{4Kt}}\, g'(p)$$

$$Q_{xx} = \frac{dQ_x}{dp}\frac{\partial p}{\partial x} = \frac{1}{4Kt}\, g''(p).$$

$$0 = Q_t - K Q_{xx} = \frac{1}{t}\left[-\frac{1}{2}\, p\, g'(p) - \frac{1}{4}\, g''(p)\right]$$

$$\Longrightarrow \quad g''(p) + 2p\, g'(p) = 0.$$

$$e^{p^2} g'' + 2p\, e^{p^2} g' = 0.$$

$$(e^{p^2} g')' = 0$$

$$e^{p^2} g' = c_1$$

$$g' = c_1 e^{-p^2}$$

$$\boxed{g(p) = c_1 \int e^{-p^2}\, dp + c_2}$$

Step 3 Select g so that ⊛ with $\phi(x) = Q(0,x)$ holds.

$$Q(t,x) = c_1 \int_0^{x/\sqrt{4kt}} e^{-p^2}\,dp + c_2 .$$

This formula is only valid for $t>0$. We use $Q(0,x)$ to get c_1, c_2.

- If $x>0$, $1 = \lim_{t\downarrow 0} Q = c_1 \int_0^{\infty} e^{-p^2}\,dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2$
- If $x<0$, $0 = \lim_{t\downarrow 0} Q = c_1 \int_0^{-\infty} e^{-p^2}\,dp + c_2 = -c_1 \frac{\sqrt{\pi}}{2} + c_2$.

$\longrightarrow c_1 = \frac{1}{\sqrt{\pi}}, \quad c_2 = \frac{1}{2} \longrightarrow$ for $t>0$.

$$\boxed{Q(t,x) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4kt}} e^{-p^2}\,dp.}$$

Step 4 We know Q. We <u>define</u> $S = \frac{\partial Q}{\partial x}$. We also define

$$\boxed{u(t,x) = \int_{-\infty}^{\infty} S(t, x-y)\,\phi(y)\,dy , \quad t>0.}$$

(By superposition + derivative property, this is a formula for a solution.)

We <u>claim</u>: u is the unique solution of ⊛.

We calculate

$$u(t,x) = \int_{-\infty}^{\infty} \frac{\partial Q}{\partial x}(t, x-y)\,\phi(y)\,dy$$

$$= -\int_{-\infty}^{\infty} \frac{\partial}{\partial y}\left[Q(t,x-y)\right]\phi(y)\,dy$$

$$= \int_{-\infty}^{\infty} Q(t,x-y)\,\phi'(y)\,dy - \underbrace{Q(t, x-y)\phi(y)\Big|_{y=-\infty}^{y=+\infty}}_{\to\, 0}$$

$$\Longrightarrow \quad u(0,x) = \int_{-\infty}^{\infty} Q(t,x-y)\,\phi'(y)\,dy\,\Big|_{t=0}$$

$$= \int_{-\infty}^{x} \phi'(y)\,dy = \phi\Big|_{-\infty}^{x} = \phi(x)$$

Thus, our formula for u provides a function which satisfies

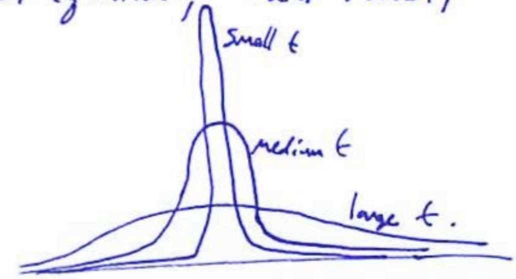
$$\lim_{t\searrow 0} u(t,x) = \phi(x).$$

We also know that $(\partial_t - \kappa\partial_x^2)u = 0$ since u is given as the superposition of $S(t,x-y) = \partial_x Q(t,x-y)$ and Q is a solution. We calculate

$$\boxed{S = \frac{\partial Q}{\partial x} = \frac{1}{2\sqrt{\pi\kappa t}}\, e^{-x^2/4\kappa t}, \quad t > 0}$$

$$\boxed{u(t,x) = \frac{1}{\sqrt{4\pi\kappa t}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\kappa t}}\,\phi(y)\,dy}$$

$S(t,x)$ is sometimes called: source function, Green's function, fundamental solution, gaussian, propagator of diffusion equation, heat kernel, diffusion kernel.



- $S : \mathbb{R}_x \times \{t > 0\} \longrightarrow \mathbb{R}$.
- $S > 0$
- S is even
- $$\int_{-\infty}^{\infty} S(t,x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-g^2}\, dg = 1 .$$ "Delta Function"

Is the solution $\phi \longmapsto U(t,x)$ we have obtained unique?

Energy-Method Proof of Uniqueness for Diffusion Equation

Suppose u_1, u_2 are two solutions solving ⊛ and emerging from same initial data ϕ. Form $w = u_1 - u_2$. By superposition, w is also a solution emerging from initial data $0 = \phi - \phi$.

Multiply diffusion equation for w by w.

$$0 = w_t - k w_{xx} \implies 0 = \left(\tfrac{1}{2} w^2\right)_t + (-k w_x w)_x + k w_x^2$$

Integrate in x:

$$0 = \int_{-\infty}^{\infty} \left(\tfrac{1}{2} w^2\right)_t dx + \cancelto{0}{\int_{-\infty}^{\infty} (-k w_x w)_x \, dx} + \int_{-\infty}^{\infty} k w_x^2 \, dx$$

$$\implies \frac{d}{dt} \int_{-\infty}^{\infty} \tfrac{1}{2} w^2(t,x)\, dx = -k \int_{-\infty}^{\infty} \left[w_x(t,x) \right]^2 dx < 0 .$$

$$\implies \int_{-\infty}^{\infty} w^2(t_1,x)\, dx \leq \int_{-\infty}^{\infty} w^2(t_2,x)\, dx \quad \text{for } t_1 > t_2$$

$$\implies w \equiv 0 .$$

Diffusion on $\mathbb{R}^3$

$$\circledast \quad \begin{cases} \partial_t u = \kappa \Delta u = \kappa \left(\partial_{x_1}^2 + \partial_{x_2}^2 + \partial_{x_3}^2\right) u \\ u(0, \underline{x}) = \phi(\underline{x}). \end{cases}$$

Theorem

$$u(t, \underline{x}) = \frac{1}{(4\pi\kappa t)^{3/2}} \iiint e^{-\frac{|\underline{x}-\underline{x}'|^2}{4\kappa t}} \phi(\underline{x}')\, d\underline{x}', \quad t > 0.$$

$(\forall\ \phi : \mathbb{R}^3 \to \mathbb{R}$ bdd., cts.$)$

Why? Set

1-d Heat Kernel

$$S_3(t, x, y, z) = S(t,x)\, S(t,y)\, S(t,z).$$

$$\partial_t S_3 = (\partial_t S)(t,x)\, S(t,y)\, S(t,z) + S(t,x)\, (\partial_t S)(t,y)\, S(t,z) + S(t,x) S(t,y) (\partial_t S)(t,z)$$

$$= (\kappa \partial_x^2 S)\, S(y)\, S(z) + S(x)\, (\kappa \partial_y^2 S)\, S(z) + S(x)\, S(y)\, (\kappa \partial_z^2 S).$$

$$= \kappa \Delta_3 S_3.$$

$\Longrightarrow S_3$ satisfies 3d heat equation.

$$\iiint S_3(t, \underline{x})\, d\underline{x} = \int S(t,x)\, dx \int S(t,y)\, dy \int S(t,z)\, dz = 1.$$

Suppose $\phi(\underline{x}) = \Phi(x)\psi(y)\zeta(z)$.

$$\lim_{t \searrow 0} \iiint S_3(t, \underline{x}-\underline{x}')\, \phi(\underline{x}')\, d\underline{x} = \lim_{t\to 0} \int S(t, x-x')\, \Phi(x')\, dx' \int S(t, y-y')\, \psi(y)\, dy' \int \dots \zeta(z')\, dz'$$

$$\oplus \qquad = \Phi(x)\, \psi(y)\, \zeta(z). = \phi(\underline{x})$$

Exercise 7.1:
- 'Justify' $\oplus$ in special case where $\phi(\underline{x}) = \Phi(x)\psi(y)\zeta(z)$.
- Prove $\lim_{t \searrow 0} \int S_3(t, \underline{x}-\underline{x}')\, \phi(\underline{x}')\, dx' = \phi(\underline{x})$ for any bounded continuous $\phi : \mathbb{R}^3 \to \mathbb{R}$.

Free Schrödinger Equation

Consider the initial value problem for free Schrödinger equation on $\mathbb{R}^3$

(we set $\hbar = m = 1$.)

$$LS(\mathbb{R}^3) \quad \begin{cases} -i\partial_t u = \frac{1}{2}\Delta u \\ u(0,x) = \phi(x) \end{cases} \qquad u: \mathbb{R}_t \times \mathbb{R}^3_x \longrightarrow \mathbb{C}.$$

This looks suspiciously similar to $\partial_t u = k\Delta u$ with $k = \frac{i}{2}$.

We are interested in solutions which tend to zero as $|x| \to \infty$.

$$\text{\$} \qquad u(t, \underline{x}) = \frac{1}{(2\pi i t)^{3/2}} \int_{\mathbb{R}^3} e^{-\frac{|\underline{x}-\underline{x}'|^2}{2it}} \phi(\underline{x}')\, d\underline{x}'.$$

This is the formula for the diffusion equation solution with $k = \frac{i}{2}$.

Note that the exponential is oscillatory, not decaying.

Exercise 7.2 Prove that the formula \$ gives a solution to $LS(\mathbb{R}3)$ for nice enough initial data ϕ.

Recall our Fourier-transform-based solution of $LS(\mathbb{R}3)$.

By Fourier inversion, we have $f(x) = \int_{\mathbb{R}^3} e^{2\pi i x\cdot\xi} \hat{\phi}(\xi)\, d\xi$.

If we define $u(t,x) = \int_{\mathbb{R}3} e^{2\pi i x\cdot\xi} e^{i w(\xi) t} \hat{\phi}(\xi)\, d\xi$ and make an appropriate choice of the dispersive function $\xi \longmapsto w(\xi)$ we will find a solution formula for $LS(\mathbb{R}3)$. Calculating $-i\partial_t$ under the integral sign spawns $w(\xi)$. Calculating $\frac{1}{2}\Delta$ spawns $\frac{1}{2}\, 2\pi i\xi \cdot 2\pi i\xi = -2\pi^2|\xi|^2$.

So, we choose $w(\xi) = -2\pi|\xi|^2$.

Thus, we also have the solution formula

$$\tilde{\mathcal{F}} \qquad u(t,x) = \int_{\mathbb{R}^3} e^{2\pi i \underline{x}\cdot\underline{\xi}}\, e^{-i2\pi^2|\xi|^2 t}\, \hat{\phi}(\xi)\, d\xi .$$

<u>Exercise 7.3</u> (a) Use Fourier transform properties to find the Fourier transform of $e^{-i|x|^2}$.

(b) Use (a) and convolution property of F.T. to show the formulas $\tilde{\mathcal{F}}$ and $\$$ define the same function.

(c) Find the formula analogous to $\tilde{\mathcal{F}}$ for the solution of the diffusion equation.

The formula $\$$ gives a <u>convolution representation</u> of the solution u of $LS(\mathbb{R}^d)$ in terms of the initial data ϕ. The formula $\tilde{\mathcal{F}}$ gives a <u>multiplier representation</u> of u in terms of $\hat{\phi}$. Each of these representations have certain advantages.

Note that $\left| e^{-i2\pi|\xi|^2 t}\, \hat{\phi}(\xi) \right| = |\hat{\phi}(\xi)| \quad \forall\, t \in \mathbb{R}$.

Thus, by Plancherel's Theorem, $\|u(t)\|_{L^2(\mathbb{R}^3)} = \|\phi\|_{L^2(\mathbb{R}^3)}$.

Based on $\$$, we instantly observe

$$\|u(t)\|_{L^\infty} \le C\, t^{-3/2}\, \|\phi\|_{L^1} .$$

By interpolation,

$$\|u(t)\|_{L^\infty} \le C t^{-3/2} \|\phi\|_{L^1}$$

$$\|u(t)\|_{L^{p'}} \le C t^{-\frac{3\theta}{2}} \|\phi\|_{L^p} \qquad \frac{1}{p} = \frac{\theta}{1} + \frac{1-\theta}{2}$$

$$\|u(t)\|_{L^2} \le C t^0 \|\phi\|_{L^2}.$$

We thus obtain a family of dispersive decay estimates for the solution.

These inequalities describe how the Schrödinger wave spreads out in space and shrinks in amplitude as time moves.

Harmonic Oscillator ; Hydrogen Atom   lecture #8

APM 421 QM

We have seen that the initial value problem for Schrödinger's equation

$$\begin{cases} i\hbar\partial_t \psi = H\psi & ; \quad H \text{ self-adjoint on } L^2 \\ \psi(0) = \psi_0 \in L^2 \end{cases}$$

is well-posed and the solution satisfies probability conservation $\|\psi(t)\|_{L^2} = \|\psi_0\|$.

We are especially interested in the situation where $H = -\frac{\hbar^2}{2m}\Delta + V(x)$ for various potentials arising from physical models. We have just completed a study of the free Schrödinger equation with $V = 0$.

A main observation we made about the dynamics of free Schrödinger waves on $\mathbb{R}^3$ is the dispersive decay estimate:

$$\|\psi(t)\|_{L^\infty(\mathbb{R}^3_x)} \leq C(1+|t|)^{-3/2} \|\psi_0\|_{L^1(\mathbb{R}^3_x)}.$$

Thus, free Schrödinger waves spread out to conserve their L^2 size while satisfying the dispersive decay.

We turn our attention to two cases involving $V \neq 0$ with a basic difference in the dynamics, namely, the existence of spatially localized solutions which do not decay with time.

Harmonic Oscillator   [Strauss ; Intro. PDEs § 9.4].

The Harmonic Oscillator Hamiltonian is $H = -\frac{\hbar^2}{2m}\Delta + \frac{1}{2}m\omega^2|x|^2$.

Let's specialize the discussion to $d=1$ and choose constants appropriately so that the equation becomes $i\partial_t u = -\partial_x^2 u + x^2 u$. We look for solutions which satisfy $u \to 0$ as $x \to \pm\infty$. This is a boundary condition "at infinity" and will be used to exclude certain solutions as "non-physical".

In today's lecture, we will not strive to solve the full initial value problem for the harmonic oscillator with general initial data ψ_0. Instead we will look for a list of solutions toward the general case.

Can we find a solution in separated form $\psi(t,x) = T(t)\,V(x)$?

$$i\dot{T}V = -TV'' + x^2 TV.$$

Divide by TV:

$$i\frac{\dot{T}}{T} = \frac{-V'' + x^2 V}{V} = -\lambda \qquad \text{for some const. } \lambda.$$

No x dependence

No t dependence

$$i\dot{T} = -\lambda T \qquad ; \qquad -V'' + x^2 V = -\lambda V.$$

$$\boxed{T(t) = C_0 e^{-i\lambda t}} \qquad \boxed{V'' + (\lambda - x^2)V = 0}$$

The ODE for V is variable coefficient so the solution is not obvious.

Consider $e^{-x^2/2}$. We calculate $(e^{-x^2/2})' = e^{-x^2/2}(-x)$. $(e^{-x^2/2})'' = e^{-x^2/2}(x^2) + e^{-x^2/2}$. Thus, $e^{-x^2/2}$ satisfies the V equation in the case $\lambda = 1$!. We are motivated by this calculation to look for solutions of the V equation of the form $V(x) = w(x)\,e^{-x^2/2}$.

$$V'(x) = w'(x)\,e^{-x^2/2} + w(x)\,e^{-x^2/2}(-x)$$

$$V''(x) = w''e^{-x^2/2} + 2w'e^{-x^2/2}(-x) + w(x)e^{-x^2/2}x^2 - w(x)\,e^{-x^2/2}.$$

Reexpress the ODE on V as an ODE on w.

$$\left[w'' + 2w'x + \underline{\underline{x^2 w}} - w\right] e^{-x^2/2} + (\lambda - \underline{\underline{x^2}})\, w e^{-x^2/2} = 0$$

$$(w'' - 2w'x - w + \lambda w)\, e^{-x^2/2} = 0$$

$$\boxed{w'' - 2w'x + (\lambda - 1) w = 0}$$

This equation is known as <u>Hermite's differential equation</u>.

We look for solutions in the form of power series:

$$w(x) = \sum_{k=0}^{\infty} a_k x^k \quad ; \quad \{a_k\}_{k=0}^{\infty} \text{ to be determined.}$$

Substituting the power series into Hermite's equation produces

$$\sum_{k=0}^{\infty} k(k-1) a_k x^{k-2} - \sum_{k=0}^{\infty} (2k - \lambda + 1) a_k x^k = 0.$$

Matching powers of x, we get

$$x^0: \quad 2a_2 + (\lambda - 1) a_0 = 0$$

$$x^1: \quad 6a_3 + (\lambda - 3) a_1 = 0, \text{ etc.}$$

$$x^k: \quad (k+2)(k+1) a_{k+2} = (2k + 1 - \lambda) a_k \qquad k = 0, 1, 2, \ldots$$

Thus, the "seed coefficients" a_0, a_1 determine the other coefficients by these recursion formula. The 1st two coefficients are arbitrary.

A simple case arises when $\lambda = 2k+1$ for some integer k. If this occurs then $a_{k+2} = 0$, $a_{k+4} = 0$ and so on. We therefore obtain a power series of finite length, also called a polynomial! Moreover, the polynomial we get is odd if k is odd and even if k is even. These are called <u>Hermite polynomials</u>:

$$H_0(x) = 1 \qquad \lambda = 1,\ a_1 = a_2 = 0$$

$$H_1(x) = 2x \qquad \lambda = 3,\ a_0 = a_3 = 0$$

$$H_2(x) = 4x^2 - 2 \qquad \lambda = 5,\ a_1 = a_4 = 0.$$

$$H_3(x) = 8x^3 - 12x \qquad \lambda = 7,\ a_0 = a_5 = 0$$

$$H_4(x) = 16x^4 - 48x^2 + 12 \qquad \lambda = 9,\ a_1 = a_6 = 0.$$

Thus, we have found some separated solutions of the time independent quantum harmonic oscillator of the form

$$V_k(x) = H_k(x)\, e^{-x^2/2} \quad \text{if } \lambda = 2k+1.$$

The corresponding solutions of time dependent problem are

$$\psi_k(t,x) = e^{-i(2k+1)t} H_k(x)\, e^{-x^2/2}.$$

Exercise 8.1 Show that all the Hermite polynomials are given by the formula

$$H_K(x) = (-1)^K e^{x^2} \frac{d^K}{dx^K} e^{-x^2}.$$

Exercise 8.2 Show directly from the Hermite equation that the functions $H_K(x) e^{-x^2/2}$ are mutually orthogonal on $(-\infty, \infty)$. That is

$$\int_{-\infty}^{\infty} H_K(x) e^{-x^2/2} H_\ell(x) e^{-x^2/2} \, dx = 0 \quad \text{if } K \neq \ell.$$

Exercise 8.3

(a) If $\lambda \neq 2K+1$ for integers K, show that any solution of Hermite's ODE is a power series but not a polynomial.

(b) Deduce that in this case no solution of Hermite's ODE can satisfy the boundary condition at ∞. (Hint: Use recursion formula to find behavior of a_K as $K \to \infty$ and compare with power series expansion of e^{x^2}.)

Hydrogen Atom [GS §7.7 ; Strauss §9.5]

A hydrogen atom consists of a proton and an electron, interacting via the Coulomb force law. We simplify the problem by assuming the proton is infinitely heavy compared to the electron. Therefore, the proton may be placed at the spatial origin and does not move. The electron moves under the influence of the Coulomb potential $V(\underline{x}) = -e^2/|\underline{x}|$ where e is the proton charge and $-e$ is the electron charge.

Thus, the Hamiltonian for the electron under these assumptions is

$$H = -\frac{\hbar^2}{2m}\Delta - e^2\frac{1}{|\underline{x}|}.$$

Let's choose $\hbar = m = e$, write $\underline{x} = (x, y, z)$ and $r = |\underline{x}| = (x^2+y^2+z^2)^{1/2}$. Thus, we are interested in finding solutions of $i\partial_t u = -\frac{1}{2}\Delta u - \frac{1}{r}u$ with the condition that $\iiint |u(t,\underline{x})|^2\, d\underline{x} < \infty$. This condition implies a vanishing as $|\underline{x}| \to \infty$.

Separate variables: $u(t,\underline{x}) = T(t)\,v(\underline{x}) \longrightarrow$ equation $\longrightarrow$

$$2i\frac{\dot{T}}{T} = \frac{-\Delta v - \frac{2}{r}v}{v} = \lambda$$

pure t dependence

pure x dependence

$$\Longrightarrow \quad u(t,\underline{x}) = e^{-i\frac{\lambda}{2}t}\, v(\underline{x}) \quad \text{where}$$

$$\boxed{-\Delta v - \frac{2}{r}v = \lambda v.}$$

Let's restrict attention further and look for spherically symmetric solutions $V(\underline{x}) = R(r)$. We thus seek R satisfying

$$\boxed{\underbrace{-R_{rr} - \frac{2}{r}R_r}_{-\Delta R} - \frac{2}{r}R = \lambda R}, \quad 0 < r < \infty$$

with the condition $\int_0^\infty |R(r)|^2 r^2 \, dr < \infty$.

We also demand that $R(0)$ is finite. The ODE that $R(\cdot)$ satisfies is another variable coefficient equation whose solutions are not obvious. This equation is known as Laguerre's Differential Equation. It turns out all the eigenvalues λ satisfy $\lambda < 0$. For now, we assume this.

Notice that, as $r \to \infty$, the $\frac{2}{r}$ prefactor decays to zero so Laguerre's equation resembles $-R_{rr} = \lambda R$ which has solutions $e^{\pm \beta r}$ where $\beta = \sqrt{-\lambda}$. The + sign choice leads to solutions which violate the L^2 finiteness condition so we toss those aside. We thus consider $e^{-\beta r}$ as an approximate solution and use it to formulate a more accurate

Ansatz:

$$w(r) = R(r)\, e^{\beta r}, \quad \beta = \sqrt{-\lambda}.$$

$$R(r) = w(r)\, e^{-\beta r}$$

$$R_r = w' e^{-\beta r} + w e^{-\beta r}(-\beta)$$

$$R_{rr} = w'' e^{-\beta r} + 2(-\beta) w' e^{-\beta r} + w e^{-\beta r} \beta^2.$$

8.8

$$\underbrace{\left(- w_{rr} + 2\beta w' + \cancel{\beta^2 w} \right) e^{-\beta r}}_{-R_{rr}} - \underbrace{\frac{2}{r}\left(w_r - \beta w \right) e^{-\beta r}}_{-\frac{2}{r} R_r} - \underbrace{\left(\frac{2}{r} + \cancel{\beta^2} \right) e^{-\beta r}}_{-\left(\frac{2}{r} - \lambda\right) R} = 0$$

$$- w_{rr} + 2\left(\beta - \frac{1}{r}\right) w_r + 2(\beta - 1)\frac{1}{r} w = 0$$

$\times -\frac{1}{2} r$

$$+ \frac{1}{2} r w_{rr} - \beta r w_r + w_r + (1-\beta) w = 0.$$

We now look for solutions in the form of a power series.

$$w(r) = \sum_{k=0}^{\infty} a_k r^k.$$

$$\frac{1}{2}\sum_{k=0}^{\infty} k(k-1) a_k r^{k-1} - \beta \sum_{k=0}^{\infty} k a_k r^k + \sum_{k=0}^{\infty} k a_k r^{k-1} + (1-\beta)\sum_{k=0}^{\infty} a_k r^k = 0.$$

change variables

$k \to k-1$

$k \to k-1.$

$$\sum_{k=0}^{\infty} \left[\frac{1}{2} k(k-1) + k \right] a_k r^{k-1} + \sum_{k=1}^{\infty} \left[-\beta(k-1) + (1-\beta) \right] a_{k-1} r^{k-1} = 0.$$

$$\Longrightarrow \frac{k(k+1)}{2} a_k = (\beta k - 1) a_{k-1}$$

$$\Longrightarrow \quad a_1 = (\beta-1)a_0 \qquad 3a_2 = (2\beta-1)a_1$$
$$6a_3 = (3\beta-1)a_2 \qquad 10a_4 = (4\beta-1)a_3$$
$$15a_5 = (5\beta-1)a_4 \qquad 21a_6 = (6\beta-1)a_5, \text{ etc.}$$

If $\beta = \frac{1}{n}$ for some $n \in \mathbb{N}$ then the sequence of coefficients eventually terminates and we get a polynomial. In this case, our solution $V(x) = w(r)\,e^{-\beta r}$, with $w(r)$ a polynomial so the decaying exponential ensures the vanishing condition at $r \to \infty$.

The eigenvalues $\lambda = -\beta^2 = -\frac{1}{n^2}$ were observed in the Balmer series and were used by Bohr to construct his model of Hydrogen. Here we see the eigenvalues arising as solvability conditions, subject to vanishing at ∞ and nonsingularity at $r=0$, for the separated ODEs.

We will relax to the nonspherically symmetric case and make a more systematic study in later lectures.

We want to classify the solutions of the Schrödinger equation

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

according to their behavior in spacetime. A basic issue is to distinguish between solutions which stay localized in space for all time and those which spread out toward spatial infinity.

Definition: The spectrum of an operator A on a Hilbert space $\mathbb{H}$ is the subset of $\mathbb{C}$ given by

$$\sigma(A) = \{ \lambda \in \mathbb{C} : A - \lambda \text{ is not invertible (has no bounded inverse)} \}.$$

The complement $\rho(A) = \mathbb{C} \setminus \sigma(A)$ is called the resolvent set of A.

For $\lambda \in \rho(A)$, the operator $(A-\lambda)^{-1}$ is well-defined.

What are the reasons why $A - \lambda$ is not invertible? The usual reasons are

1. $(A-\lambda)\psi = 0$ has a nonzero solution $\psi \in \mathbb{H}$. In this case, λ is called an eigenvalue and ψ a corresponding eigenvector or eigenfunction.
2. $(A-\lambda)\psi = 0$ "almost" has a nonzero solution. More precisely, we say $\{\psi_n\} \subset \mathbb{H}$ is a Weyl sequence for A and λ if
   a) $\|\psi_n\| = 1 \quad \forall n$
   b) $\|(A-\lambda)\psi_n\| \longrightarrow 0$ as $n \longrightarrow \infty$.
   c) $\psi_n \longrightarrow 0$ weakly as $n \to \infty$. (This means $\langle \phi, \psi_n \rangle \to 0 \ \forall \phi \in \mathbb{H}$.)

Definition The discrete spectrum of an operator A is

$$\sigma_d(A) = \{ \lambda \in \mathbb{C} : \lambda \text{ is an isolated eigenvalue of } A \text{ w. finite multiplicity} \}$$

isolated: $\exists$ Nbhd $\ni \lambda$ s.t. Nbhd $\cap\, \sigma(A) = \phi$.

multiplicity: $\text{Null}(A-\lambda) = \{ v \in \mathbb{H} : (A-\lambda)v = 0 \}$.

multiplicity of λ = dimension $(\text{Null}(A-\lambda))$.

Problem 9.1 1. Show $Null\,(A-\lambda)$ is a vector space

2. Show that if $A = A^*$, eigenvectors of A corresponding to different eigenvalues are orthogonal.

Definition: The <u>essential spectrum</u> of the operator A is all of the spectrum outside the discrete spectrum:

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

Remark: The terms point spectrum / continuous spectrum are sometimes used in place of discrete spectrum / essential spectrum, respectively.

We'd like to distinguish $\sigma_d(A)$ from $\sigma_{ess}(A)$ if possible.

Definition The <u>Weyl spectrum</u> of an operator A is

$$\sigma_w(A) = \{\lambda : \exists \text{ weyl sequence for } A \text{ and } \lambda\}.$$

Weyl's Theorem If $A = A^*$ then $\sigma_{ess}(A) = \sigma_w(A) \Longrightarrow$ $\sigma(A) = \sigma_d(A) \cup \sigma_{ess}(A)$ + $\sigma_d(A) \cap \sigma_{ess}(A) = \phi$.

proof Suppose $\lambda \in \sigma_{ess}(A)$. Then $\inf_{\substack{\|\psi\|=1 \\ \psi\in D(A)}} \|(A-\lambda)\psi\| = 0$. Otherwise, $A-\lambda$ invertible. $Null\,(A-\lambda) = \{0\}$ and $Range\,(A-\lambda) = \mathbb{H} \Longrightarrow$ But $\lambda \in \sigma(A)$ so that is not possible. Thus, $\exists$ sequence $\{\psi_n\} \subset D(A)$ s.t. $\|\psi_n\| = 1$ and $\|(A-\lambda)\psi_n\| \to 0$ as $n \to \infty$. By Banach-Alaoglu theorem $\exists$ subsequence $\{\psi_{n'}\} \subset \{\psi_n\}$ and an element $\psi_0 \in \mathbb{H}$ s.t. $\psi_n \rightharpoonup \psi_0$ weakly as $n \to \infty$. (Drop the n' in favor of n for now.) This implies $\forall\, f \in D(A)$ that

$$\langle (A-\lambda) f, \psi_0\rangle = \lim_{n\to\infty} \langle (A-\lambda) f, \psi_n\rangle = \lim_{n\to\infty} \langle f, (A-\lambda)\psi_n\rangle = 0.$$

This implies $\psi_0 \in D(A)$. Since $D(A) = D(A^*) = \{\psi \in \mathbb{H} : \langle Af, \psi\rangle \le C\|f\|\ \forall f \in D(A)\}$ and $|\langle Af, \psi_0\rangle| = |\lambda \langle f, \psi_0\rangle| \le |\lambda|\, \|\psi_0\|\, \|f\|$ and $A\psi_0 = \lambda\psi_0$.

If $f_0 = 0$ then f_n is a Weyl sequence for A and λ so $\lambda \in \sigma_W(A)$. 9.3

If $f_0 \neq 0$ then λ is an eigenvalue of A. Since $\lambda \in \sigma_{ess}(A)$, λ must either have infinite multiplicity or be nonisolated.

- If λ has infinite multiplicity then consider an orthonormal basis of $\mathrm{Null}(A-\lambda)$. The basis functions form a Weyl sequence for A and λ so $\lambda \in \sigma_W(A)$.
- If λ is nonisolated then consider $\lambda_j \in \sigma(A) \setminus \{\lambda\}$ with $\lambda_j \to \lambda$.
  - If $\exists$ subsequence corresponding to distinct eigenvalues, the corresponding sequence of normalized eigenfunctions is orthonormal and converges weakly to zero so forms a Weyl sequence for A and $\lambda \Rightarrow \lambda \in \sigma_W(A)$.
  - If the sequence λ_j consists (eventually) of non-eigenvalues then, arguing as before for each λ_j, we can construct a diagonal sequence of functions which form a Weyl sequence for A and λ. $\Longrightarrow \lambda \in \sigma_W(A)$. We have just shown $\sigma_{ess}(A) \subset \sigma_W(A)$.

Now suppose $\lambda \in \sigma_W(A)$ and let $\{f_n\}$ be corresponding Weyl sequence. Then we have $\lambda \in \sigma(A)$ since otherwise

$$\|f_n\| = \|(A-\lambda)^{-1}(A-\lambda)f_n\| \le \|(A-\lambda)^{-1}\|\,\|(A-\lambda)f_n\| \to 0.$$

(c!).

Suppose λ is an isolated eigenvalue of finite multiplicity, so $\lambda \in \sigma_d(A)$. Suppose the multiplicity is one (other cases are similar). Let f_0 be the corresponding normalized eigenvector. Write $f_n = c_n f_0 + \tilde{f}_n$ with $c_n = \langle f_0, f_n \rangle$ and $\langle \tilde{f}_n, f_0 \rangle = 0$. Since $f_n \to 0$ weakly, we must have $c_n \to 0$ so $\|\tilde{f}_n\| \to 1$. Also $(A-\lambda_n)\tilde{f}_n \to 0$. Because λ is isolated in the spectrum, $(A-\zeta)^{-1}$ is uniformly bounded on $(f_0)^\perp$ for ζ near λ so $\|\tilde{f}_n\| = \|(A-\lambda)^{-1}(A-\lambda_n)\tilde{f}_n\| \le (\text{const})\,\|(A-\lambda_n)\tilde{f}_n\| \to 0$ which is a contradiction. Thus $\lambda \in \sigma_{ess}(A)$ showing $\sigma_W(A) \subset \sigma_{ess}(A)$.

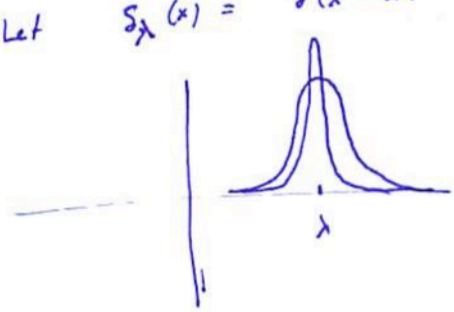
Problem 9.2 Show that if $U : \mathcal{H} \to \mathcal{H}$ is unitary then $\sigma(U^* A U) = \sigma(A)$, $\sigma_d(U^* A U) = \sigma_d(A)$ and $\sigma_{ess}(U^* A U) = \sigma_{ess}(A)$.

Example Spectrum of the operators x_j and P_j on $L^2(\mathbb{R}^d)$.

1. $\sigma(P_j) = \sigma_{ess}(P_j) = \mathbb{R}$.
2. $\sigma(x_j) = \sigma_{ess}(x_j) = \mathbb{R}$.

proof of 2. Suppose, for simplicity, $d=1$: For any $\lambda \in \mathbb{R}$ we find a sequence of functions $\{\psi_n\} \subset \mathcal{H}$ s.t. $\|\psi_n\| = 1$ $\forall n$ and $\|(x_j - \lambda)\psi_n\| \to 0$ as $n \to \infty$ and $\psi_n \to 0$ weakly as $n \to \infty$. Thus, we construct a Weyl sequence for x_j and λ. We build this sequence by approximating dirac mass.

Let $\delta_\lambda(x) = \delta(x-\lambda)$ be the delta-function which satisfies $(x-\lambda)\delta_\lambda = 0$.



We will construct a sequence approximating δ_λ.

Let $\phi \in C_0^\infty(-1,1)$ such that $\phi \geq 0$ and $\int |\phi|^2 = 1$. Now translate and rescale ϕ by writing

$\psi_n(x) = n^{1/2} \phi(n[x-\lambda])$.

The choice of scaling guarantees $\int |\psi_n(x)|^2 dx = 1$ $\forall n$, and

$\|(x-\lambda)\psi_n\|_{L^2}^2 = \int |x-\lambda|^2 n |\phi(n(x-\lambda))|^2 dx = \frac{1}{n^2}\int |y|^2 |\phi(y)|^2 dy \to 0$ as $n \to \infty$.

We now show $\psi_n \to 0$ weakly as $n \to \infty$.

Thus, $\lambda \in \sigma(x)$.

$\forall f \in L^2(\mathbb{R}^d)$, $\left|\int \bar{\psi}_n f\right| = \left|\int_{|x-\lambda| < \frac{1}{n}} \bar{\psi}_n f\right| \leq \left(\int |\psi_n|^2\right)^{\frac{1}{2}} \left(\int_{|x-\lambda| \leq \frac{1}{n}} |f|^2\right)^{\frac{1}{2}} \to 0$.

Thus, $\lambda \in \sigma_{ess}(x)$. It is easy to see that x has no eigenvalues.

$(x\psi = \lambda\psi \iff (x-\lambda)\psi = 0 \Rightarrow x = \lambda$ at all points where $\psi \neq 0)$ C!

proof of 1.

We seek a Weyl sequence $\{f_n\}$ for p and λ. By F.T. properties, we have

$\| (p-\lambda) f_n \| = \| [(p-\lambda) f_n]^\wedge \| = \| (k-\lambda) \hat{f}_n \|$.

Take for $f_n = n^{1/2} \hat{\phi}(n(k-\lambda))$ for $\hat{\phi}$ supported on $[-1,1]$, with $\int |\hat{\phi}|^2 dk = 1$. So $\|f_n\| = \|\hat{f}_n\| = 1$ and $\int \bar{f} f_n = \int \hat{\bar{f}} \hat{f}_n \to 0 \ \forall f \in L^2$.

Moreover, $\| (k-\lambda)\hat{f}_n \| \to 0 \Rightarrow \|(p-\lambda) f_n\| \to 0$ so f_n is Weyl for p and λ. Thus $\sigma(p) = \sigma_{ess}(p) = \mathbb{R}$. Let us see what f_n looks like. We have

$f_n(x) \equiv (2\pi\hbar)^{-1/2} \int e^{ix\cdot k/\hbar} n^{1/2} \hat{f}(n(x-\lambda))\, dk = e^{ix\cdot\lambda/\hbar} n^{-1/2} \phi(x/n)$.

Suppose $f \equiv 1$ for $|x| \le \frac{1}{2}$ then f_n looks like a plane wave (amplitude $n^{-1/2}$ and wave vector λ), cutoff near ∞ by $\phi(x/n)$.

The proof that $\sigma(P_j) = \sigma_{ess}(P_j) = \mathbb{R}$ also follows directly from proof that $\sigma(x_j) = \sigma_{ess}(x_j) = \mathbb{R}$ w. F.T. properties ∎

Problem 9.3 Prove.

1. For $V: \mathbb{R}^d \to \mathbb{C}$ cts, the spectrum of corresponding multiplication operator on $L^2(\mathbb{R}^d)$ is $\sigma(V) = \overline{\text{range}(V)}$.
2. On $L^2(\mathbb{R}^d)$, $\sigma(-\Delta) = \sigma_{ess}(-\Delta) = [0,\infty)$.

Note: $A = A^* \Longrightarrow \sigma(A) \subset \mathbb{R}$.

Proposition. Let A be self-adjoint on $\mathcal{H}$. If λ is an accumulation point of the spectrum $\sigma(A)$ then $\lambda \in \sigma_{ess}(A)$.

proof. Suppose $\lambda_j \in \sigma(A)$ and $\lambda_j \to \lambda$ as $j \to \infty$. Then we can find $\psi_j \in D(A)$ with $\|\psi_j\| = 1$ and satisfying $\|(A-\lambda_j)\psi_j\| \leq \frac{1}{j}$ by the Weyl criterion. Since

$$\|(A-\lambda)\psi_j\| \leq \|(A-\lambda_j)\psi_j\| + |\lambda - \lambda_j| \to 0 \quad \text{as } j \to \infty$$

we see that $\lambda \in \sigma(A)$ (either $\psi_j \to 0$ weakly as $j \to \infty$ so $\lambda \in \sigma_{ess}(A)$ or else λ is an eigenvalue of A). Since λ is an accumulation point of $\sigma(A)$ it is not isolated so $\blacksquare$

$\lambda \notin \sigma_d(A) \implies \lambda \in \sigma_{ess}(A)$.

Functions of Operators and the spectral mapping theorem

Problem 9.4 Let A be a bounded self-adjoint operator. Show $\sigma(A) \subset [-\|A\|, \|A\|]$. Hint: use that if $|z| > \|A\|$ then $\|(A-z)u\| \geq (|z| - \|A\|)\|u\|$.

Suppose $f(\lambda)$ is analytic in a complex disk of radius R, $\{\lambda \in \mathbb{C} : |\lambda| < R\}$, with $R > \|A\|$. So f has a power series expansion $f(\lambda) = \sum_{n=0}^{\infty} a_n \lambda^n$ which converges $\forall\ |\lambda| < R$. Define the operator $f(A) = \sum_{n=0}^{\infty} a_n A^n$. (We've seen this w. e^A before...).

Another example: $f(\lambda) = (\lambda - z)^{-1}$ for $|z| > \|A\|$ is analytic

Weyl Criterion proof from [GS] is incomplete and confused!

$\lambda \in \sigma_{ess}(A) \Rightarrow \lambda \in \sigma_w(A)$.

Since $A-\lambda$ is not bounded invertible $\exists \{\psi_n\} \subset D(A)$ s.t.
$\|\psi_n\| = 1$ and $\|(A-\lambda)\psi_n\| \to 0$ as $n \to \infty$.
Banach-Alaoglu $\Rightarrow \exists \{\psi_{n'}\} \subset \{\psi_n\}$ and $\psi_0 \in \mathbb{H}$ s.t.
$\psi_n \to \psi_0$ weakly in H. Drop n'.

(*) $\forall f \in D(A)$ ...

$$\langle (A-\lambda)f, \psi_0 \rangle = \lim_{n\to\infty} \langle (A-\lambda) f, \psi_n \rangle \to 0.$$

$\Rightarrow \psi_0 \in D(A)$!

If $\psi_0 = 0$ then ψ_n is Weyl sequence (DONE).

If $\psi_0 \neq 0$ Then we still need to build the Weyl Sequence. Here we have an eigenfunction to with eigenvalue $\lambda \in \sigma_{ess}(A)$ so either we have

- $\dim(\mathrm{Null}(A-\lambda)) = \infty$

or

- $\exists \lambda_j \to \lambda$ with $\lambda_j \in \sigma(A)$.
  - λ_j' all eigenvalues $\to$ Weyl Sequence
  - λ_j eventually no eigenvalues!

This means that

$(A - \lambda_j)$ is not boundedly invertible.

$\Longrightarrow$ $\exists$ $\{\psi_n^j\}$ as in $\circledast$ and $\exists$ limit object f_0^j. If $f_0^j \neq 0$ we have an eigenfunction so this does not occur.

Hence $f_0^j = 0$.

Now define $\psi^j_{n(j)}$ such that $\|(A - \lambda_j)\, f^j_{n(j)}\| \leq \frac{1}{j}$ and $\forall\ f \in \mathbb{H}$,

and proceed. $\langle \psi^j_{n(j)}, f \rangle \leq \frac{1}{j}$.

Diagonalization can depend upon f. ?

not allowed ?

Where is the uniformity . . .

$\forall\ \dot{\imath}$

Use separability ?

We follow some lecture notes of R. Jerrard which are based on [Riesz - Sz. Nagy].

Spectral Theorem for bounded self-adjoint operators on $\mathbb{H}$

- $A : \mathbb{H} \to \mathbb{H}$, bdd, self-adjoint.
- Assume that $mI \le A \le \mathcal{M} I$ $\quad (\Leftrightarrow m\|\psi\|^2 \le \langle \psi, A\psi \rangle \le \mathcal{M}\|\psi\|^2 \ \forall \psi \in \mathbb{H})$

for some $-\infty < m \le \mathcal{M} < +\infty$.

$\Rightarrow \exists$ unique family $\{E_\lambda\}_{\lambda \in \mathbb{R}}$ of orthogonal projection operators s.t.

$$* \quad E_\lambda E_\mu = E_\mu E_\lambda = E_\lambda \quad \text{for } \lambda \le \mu$$

$$* \quad E_\lambda = \underset{\mu \searrow \lambda}{s\text{-}\lim}\, E_\mu$$

$$* \quad E_\lambda = 0 \text{ for } \lambda < m, \quad E_\lambda = I \text{ for } \lambda \ge \mathcal{M}$$

and if $u : (m - \delta, \mathcal{M}) \to \mathbb{C}$ is continuous (for some small $\delta > 0$)

then
$$u(A) = \int_{m-\delta}^{\mathcal{M}} u(\lambda)\, dE_\lambda .$$

Remarks:

- For bounded operators $A = \underset{\sigma \to \sigma_0}{s\text{-}\lim}\, A_\sigma$ means $\|A_\lambda \psi - A\psi\| \to 0 \ \forall \psi \in H$ as $\lambda \to \sigma_0$.
- The integral defining $u(A)$ is a Stieltjes integral with the implied limit taken in the operator norm. The lower limit of integration $m - \delta < m$ so the associated partitions used to define the integral start at some $\lambda_0 < m$. The choice $u(A) = A$ corresponding to $u(\lambda) = \lambda$ gives a spectral family representation of the operator A.
- The formula for $u(A)$ provides a homomorphism from {cts. functions: $u : (m-\delta, \mathcal{M}] \to \mathbb{C}$} $\longrightarrow$ {operators $U : \mathbb{H} \to \mathbb{H}$ given by formula $u(A)$}. This homomorphism is called the "functional calculus" and is a key output of the spectral theorem.

More on the Stieltjes integral

What does $\int_a^b \lambda \, dE_\lambda$ mean ?

Let P denote a partition of $[a,b]$: $a=\lambda_0 < \lambda_1 < \cdots < \lambda_K = b$.

Let $|P|$ denote mesh size so $|P| = \max_i |\lambda_i - \lambda_{i-1}|$. Let $\mu_i \in [\lambda_{i-1}, \lambda_i]$.

Then

$$\int_a^b \lambda \, dE_\lambda = \lim_{|P| \to 0} \sum \mu_i (E_{\lambda_i} - E_{\lambda_{i-1}}).$$

Implicitly we are asserting this limit exists and is independent of the sequence of partitions we use to define it or the choices of $\mu_i \in [\lambda_{i-1}, \lambda_i]$ whenever we write $\int_a^b \lambda \, dE_\lambda$.

The convergence of the limit is in the operator norm sense.

Exercise 10.1 (summation by parts)

Define appropriate functions so that the summation by parts formula below may be understood as integration by parts for a Stieltjes integral:

Suppose $\{f_k\}$, $\{g_k\}$ are sequences. Then

$$\sum_{k=m}^{n} f_k (g_{k+1} - g_k) = [f_{n+1} g_{n+1} - f_m g_m] - \sum_{k=m}^{n} g_{k+1} (f_{k+1} - f_k)$$

<u>Lemma 1</u> $\left.\begin{array}{l} A : \mathbb{H} \to \mathbb{H} \text{ bounded} \\ \langle A\psi, \psi\rangle \in \mathbb{R} \ \forall \psi \in \mathbb{H} \end{array}\right\} \Rightarrow A$ is symmetric.

<u>proof</u>. We are given that $\langle A\eta, \eta\rangle \in \mathbb{R}$ $\forall \eta \in \mathbb{H}$. Write $\eta = \psi + \lambda\phi$ and expand:

$$\langle A(\psi + \lambda\phi), (\psi + \lambda\phi)\rangle = \underbrace{\langle A\psi, \psi\rangle}_{\in \mathbb{R}} + |\lambda|^2 \underbrace{\langle A\phi, \phi\rangle}_{\in \mathbb{R}.} + \langle A\psi, \lambda\phi\rangle + \langle \lambda A\phi, \psi\rangle$$

$$\Rightarrow \langle A\psi, \lambda\phi\rangle + \langle \lambda A\phi, \psi\rangle = \overline{\langle A\psi, \lambda\phi\rangle + \langle \lambda A\phi, \psi\rangle}.$$

$$\lambda\langle A\psi, \phi\rangle + \bar{\lambda}\langle A\phi, \psi\rangle = \langle \lambda\phi, A\psi\rangle + \langle \psi, \lambda A\phi\rangle$$

$$= \bar{\lambda}\langle \phi, A\psi\rangle + \lambda\langle \psi, A\phi\rangle.$$

The only way this can be true for all λ is that $\langle A\psi, \phi\rangle = \langle \phi, A\psi\rangle$.

Thus, A is symmetric. ∎

<u>Lemma 2</u> $A : \mathbb{H} \to \mathbb{H}$ bounded, symmetric $\Rightarrow \sup_{\|\psi\|=1} \langle A\psi, \psi\rangle = \sup_{\|\psi\|=1} \|A\psi\|$.

<u>proof</u>: $\langle A\psi, \psi\rangle \le \|A\|$ whenever $\|\psi\| \le 1$ follows from Cauchy-Schwarz.

The other inequality follows once one observes: $\forall \lambda \in \mathbb{R}$

$$\|A\psi\|^2 = \frac{1}{4}\left[\left\langle A\left(\lambda\psi + \frac{A\psi}{\lambda}\right), \lambda\psi + \frac{A\psi}{\lambda}\right\rangle - \left\langle A\left(\lambda\psi - \frac{A\psi}{\lambda}\right), \lambda\psi - \frac{A\psi}{\lambda}\right\rangle\right]$$

Let $N_A = \sup_{\|\psi\|=1} |\langle A\psi, \psi\rangle|$. Then the right side is bounded by

$$\le \frac{1}{4}\left(N_A \left\|\lambda\psi + \frac{A\psi}{\lambda}\right\|^2 + N_A\left\|\lambda\psi - \frac{A\psi}{\lambda}\right\|^2\right) = \frac{1}{2} N_A\left(\lambda^2\|\psi\|^2 + \frac{\|A\psi\|^2}{\lambda^2}\right)$$

Now, set $\lambda^2 = \|\psi\|^{-1}\|A\psi\|$ to obtain

$$\|A\psi\|^2 \le N_A\left(\|\psi\|\,\|A\psi\|\right) \Rightarrow \|A\psi\| \le N_A\|\psi\|$$ as claimed. ∎

<u>Note</u>: If $mI \le A \le \underline{M}I$ then $\|A\| \le \max\{-m, \underline{M}\} \le \max\{|m|, |\underline{M}|\}$.

Lemma 3

$$\left.\begin{array}{l} \{A_n\}_{n=1}^{\infty} \text{ sequence} \\ A_n : \mathbb{H} \to \mathbb{H} \text{ bounded, symmetric} \\ mI \le A_n \le A_{n+1} \le MI \quad \forall n \end{array}\right\} \Rightarrow \begin{array}{l} \exists\ A : \mathbb{H} \to \mathbb{H} \text{ bounded, symmetric} \\ \operatorname{s-lim}_{n\to\infty} A_n = A. \end{array}$$

proof: Suppose $B : \mathbb{H} \to \mathbb{H}$ and $B \ge 0$. Then $\forall \lambda$ we have

$\langle B(\psi - \lambda\phi), \psi - \lambda\phi \rangle \ge 0 \Longrightarrow$ generalized Cauchy-Schwarz:

$\langle B\psi, \phi \rangle \le \langle B\psi, \psi \rangle^{1/2} \langle B\phi, \phi \rangle^{1/2} \quad \forall\ \phi, \psi \in \mathbb{H}$ when $B \ge 0$.

The monotonicity assumption implies $A_n - A_m \ge 0$ whenever $m \le n$. Thus, $\forall\ \phi \in \mathbb{H}$

$$\langle (A_n - A_m)\psi, \phi \rangle^2 \le \langle (A_n - A_m)\psi, \psi \rangle \langle (A_n - A_m)\phi, \phi \rangle.$$

In particular, this inequality is true if we choose $\phi = (A_n - A_m)\psi$ so

$$\|(A_n - A_m)\psi\|^4 \le \langle (A_n - A_m)\psi, \psi \rangle \langle (A_n - A_m)^2\psi, (A_n - A_m)\psi \rangle.$$

$$\le \langle (A_n - A_m)\psi, \psi \rangle \|A_n - A_m\|^3 \|\psi\|^2.$$

The sequence of operators $A_n - A_m$ satisfies $0 \le A_n - A_m \le (M - m)I$

so, by Lemma 2 (see Note following proof) $\|A_n - A_m\| \le M - m$.

The assumptions imply $\langle A_n\psi, \psi \rangle$ is a bounded monotone increasing sequence of real numbers, hence it is convergent. We thus observe that $A_n\psi$ is a Cauchy sequence in $\mathbb{H}$. This defines $A\psi$. ∎

<u>Lemma 4</u> $\left.\begin{array}{l} A: \mathbb{H} \to \mathbb{H}, \text{ bounded, symmetric} \\ A \geq 0 \end{array}\right\} \Rightarrow \exists!\ \sqrt{A}: \mathbb{H} \to \mathbb{H}$ s.t.

- $\sqrt{A} \geq 0$
- $(\sqrt{A})^2 = A$

Moreover, $\sqrt{A}$ commutes w. every operator that commutes with A.

<u>proof</u> We may assume $0 \leq A \leq I$. To construct a solution $X = \sqrt{A}$ of the equation $X^2 = A$ we look for $Y = I - X$. We will write $B = I - A$. The equation $X^2 = A$ translates to $(I + Y)^2 = I - B \Leftrightarrow Y = \frac{1}{2}(Y^2 + B)$. If we can find Y from B, we will have found X from A.

We define a sequence of operators $\{Y_n\}$ by iteration:

$$\begin{cases} Y_0 = 0 \\ Y_{n+1} = \frac{1}{2}(Y_n^2 + B). \end{cases}$$

Let's calculate: $Y_1 = \frac{1}{2}B$, $Y_2 = \frac{1}{2}\left((\frac{1}{2}B)^2 + B\right)$ so $Y_n = g_n(B)$ for some sequence of polynomials $\{g_n\}$. The polynomials satisfy

$g_{n+1}(x) = \frac{1}{2} g_n^2(x) + x.$ Note that $g_{n+1}(x) - g_n(x) = \frac{1}{2}(g_n - g_{n-1})(g_n + g_{n-1})$

<u>Claim</u>: The polynomials g_n have nonnegative coefficients for every n.

True for g_1, g_2. Note that $g_2 - g_1$ is also a polynomial with nonnegative coefficients. Therefore $g_3 - g_2 = \frac{1}{2}(g_2 - g_1)(g_1 - 0)$ has nonnegative coefficients. Hence, by induction $g_{n+1} - g_n$ has nonnegative coefficients for all n. Adding g_n to this produces a polynomial also w. nonnegative coefficients so g_{n+1} has nonnegative coefficients.

we thus have $Y_{n+1} \geq Y_n$ for every n. We also have $Y_n \leq I$ for every n since $B \leq I$.

By Lemma 3 there exists $Y := \text{s-}\lim_{n \to \infty} Y_n$ which satisfies $Y = \frac{1}{2}(Y^2 + B)$. Therefore $\sqrt{A} = X = I - Y$ solves $X^2 = A$. Since $\sqrt{A}$ is built as a limit of polynomials of A, it commutes with all operators that commute with A. $\blacksquare$

We omit the proof of uniqueness.

__Lemma 5__
$$\left.\begin{array}{l} A, B : \mathbb{H} \to \mathbb{H} \text{ bounded, symmetric} \\ A \geq 0,\ B \geq 0 \\ AB = BA \end{array}\right\} \implies AB \geq 0.$$

__proof__:
$$\langle AB\psi, \psi \rangle = \langle \sqrt{A}\sqrt{A} B\psi, \psi \rangle = \langle \sqrt{A} B\psi, \sqrt{A}\psi \rangle = \langle B\sqrt{A}\psi, \sqrt{A}\psi \rangle \geq 0$$
since $B \geq 0$.

__Proposition__ $A : \mathbb{H} \to \mathbb{H}$ bounded, symmetric. $m I \leq A \leq M I$.
$C_u(m, M) = \{$ upper semicontinuous functions on $[m, M]\}$.
$\forall\, u \in C_u(m, M)$ $\exists !$ bounded symmetric operator $u(A)$ s.t. $\forall\, u, v \in C_u(m, M)$ $\forall\, a \in \mathbb{R}$, the map $u \mapsto u(A)$ is:

- homogeneous $(au)(A) = a\,u(A)$
- additive $(u+v)(A) = u(A) + v(A)$
- multiplicative $(uv)(A) = u(A)\,v(A)$
- monotone $u \geq v \implies u(A) \geq v(A)$

Finally, $u \mapsto u(A)$ is cts in two senses:

① $u_n(x) \searrow u(x)$ $\forall\, x \in [m, M] \implies u(A) = \text{s-}\lim_{n \to \infty} u_n(A)$

② $\|u(A)\| \leq \max_{x \in [m, M]} |u(x)|$. (If $u_n \to u$ uniformly on $[m, M]$ then $\lim_{n \to \infty} \|u(A) - u_n(A)\| = 0$.)

proof.

1. Suppose u, v are polynomial functions. Observe that homogeneity, additivity, multiplicativity are obvious. We turn our attention to monotonicity.
Any polynomial p with real coefficients which is nonnegative on $[m, M]$ can be factored as

$$p(\lambda) = c\,(\lambda - a_1) \cdots (\lambda - a_j)\,(b_1 - \lambda) \cdots (b_k - \lambda)\, g_1(\lambda) \cdots g_\ell(\lambda)$$

with $c \geq 0$, $a_i \leq m$ and $b_i \geq M$ and g_i a nonnegative quadratic for all i.
The point is that there can be no real roots of odd multiplicity in the interval $[m, M]$. Secondly, if z_i is a complex root then so is $\bar{z}_i$ so $g_i(\lambda) = (\lambda - z_i)(\lambda - \bar{z}_i)$ is a nonnegative quadratic.

Thus, we observe that any polynomial $p(x) \geq 0$ $\forall x \in [m, M]$ induces an operator $p(A) = c\,(A - a_i I)(b_i I - I)\, g_i(A) \geq 0$, provided $m \leq A \leq M$.

2. $u: \mathbb{R} \to \mathbb{R}$ is <u>upper semicontinuous</u> if $u(x) \geq \limsup_{y \to x} u(y)$ $\forall x \in \mathbb{R}$.
By the (nontrivial) Stone-Weierstrass theorem from real analysis, ~~states~~ we know that $\forall u \in C_u(m, M)$ $\exists$ sequence of polynomials $g_n(x)$ which decreases monotonically to $u(x)$ as $n \to \infty$ $\forall x \in [m, M]$.

3. Thus, given $u \in C_u(m, M)$ $\exists$ sequence of polynomials $g_n(x)$ decreasing monotonically to $u(x)$ $\forall x \in [m, M]$. It follows that $g_n(A)$ is a monotonically decreasing sequence of operators. By Lemma 3 (also works for decreasing sequences) we can find the limit of this sequence and can see the limit is independent of the chosen sequence. This defines $u(A)$.

4. The remaining claims are straightforward. The second continuity assertion ② uses Lemma 2.

proof of spectral theorem

Define $e_\lambda(x) = \begin{cases} 1 & x \le \lambda \\ 0 & \text{otherwise.} \end{cases}$ Next, define $E_\lambda = e_\lambda(A)$.

This definition makes sense in light of the Proposition. It is obvious that $e_\lambda e_\mu = e_\mu e_\lambda = e_{\min\{\mu, \lambda\}}$ and the multiplicative property of Proposition 1 lifts this to the operator setting of E_λ.

Similarly, $e_\lambda = \lim_{\mu \searrow \lambda} e_\mu$ and this lifts.

It remains to verify the spectral family representation formula. Fix a continuous function u. Fix a partition $P: \lambda_0 < m \le \lambda_1 < \cdots < \lambda_N$ with $\lambda_N \ge M$ and fix $\mu_i \in [\lambda_i, \lambda_{i+1}]$. We define

$$u_p(\lambda) = \sum_{i=0}^{M} u(\mu_i)\left[e_{\lambda_{i+1}}(\lambda) - e_{\lambda_i}(\lambda)\right].$$

By definition, this sum is an approximating sum for the Stieltjes integral.

Moreover,

$$\|u_p(A) - u(A)\| \le \max_{\lambda \in [m, M]} |u_p(\lambda) - u(\lambda)|$$

$$= \max_{\lambda \in [m, M]} \left| \sum_{i=0}^{M} u(\mu_i) - u(\lambda)\left[e_{\lambda_{i+1}}(\lambda) - e_{\lambda_i}(\lambda)\right] \right|$$

$$\le \max_{\lambda \in [m, M]} \sum_{i=0}^{M} |u(\mu_i) - u(\lambda)| \left[e_{\lambda_{i+1}}(\lambda) - e_{\lambda_i}(\lambda)\right]$$

$$\le \max_i \max_{\lambda_i \le \lambda \le \lambda_{i+1}} |u(\mu_i) - u(\lambda)|. \quad \text{(telescope)}$$

Since u is cts., this quantity tends to zero as the partition is refined.

We omit the proof of uniqueness of the formula for $u(A)$.