(1) Introduction The stability of matter

- QM solves one of the problems of CM: why does matter not collapse onto itself, why do atoms exist?
- CM of one particle: State given by a point $(x, p) \in \mathbb{R}^6$
  position x; momentum $p = mv$, mass m

dynamics (time evolution): system of ODEs:

$$\dot{x} = \frac{\partial H}{\partial p} \quad ; \quad \dot{p} = -\frac{\partial H}{\partial q} \qquad (1)$$

where $H = H(x, p)$ is the Hamiltonian, given by physics.

Ex: particle in a force field $F(x) = -\nabla V(x)$, typically electric force

$$V(x) \propto \frac{1}{|x|} \qquad \text{"Coulomb potential"}$$

$$H(x, p) = \frac{1}{2m} p^2 + V(x)$$

Then (1) yield Newton's equation $m\ddot{x} = F(x)$.
Other forces can be incorporated: Lorentz force in a magnetic field $-p \wedge B(x)$ implemented by minimal coupling $p \mapsto p + \frac{e}{c} A(x)$ where $A(x)$ is such that $\operatorname{curl} A = B$.

$$H(x, p) = \frac{1}{2m}\left(p + \frac{e}{c} A(x)\right)^2 + V(x)$$

- CM of N particles: state given by a point $(x_1, \dots, x_N, p_1, \dots, p_N) \in \mathbb{R}^{6N}$

Ex: N electrons, M fixed nuclei at $R_1, \dots, R_M$ with Coulomb interactions

* Potential energy
$V(\underline{x}, \underline{R}) = e^2 \left(W(\underline{x}, \underline{R}) + I(\underline{x}) + U(\underline{R}) \right)$
where
$$W(\underline{x}, \underline{R}) = -\sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j}{|x_i - R_j|}$$ ← nuclear charge, attractive
(electrons – nuclei)

$$I(\underline{x}) = \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|}$$ repulsive electron-electron interaction
$$U(\underline{R}) = \sum_{1 \le i < j \le M} \frac{Z_i Z_j}{|R_i - R_j|}$$ repulsive interaction between nuclei

* Kinetic energy $T(\underline{p}) = \sum_{i=1}^{N} \frac{1}{2m} p_i^2$
(nuclei are fixed with formal limit $m_{nucl.} \to \infty$

* Magnetic fields can be taken into consideration

⇝ Full microscopic model of atoms and molecules

Problem: The equilibrium state of such a system, at fixed $R_1, \dots, R_M$, is given by $(\underline{x}, \underline{p}) \in \mathbb{R}^{6N}$ that minimizes the Hamiltonian.
But $H = T + V$ is an unbounded function on $\mathbb{R}^{6N}$ and indeed the electrons would all collapse onto the nuclei.

Quantum mechanics solves this problem and through rather simple mathematics.
→ Stability of matter.

- QM of one particle in $\mathbb{R}^3$. The state of CM must be replaced by a function

$$\mathbb{R}^3 \ni x \mapsto \psi(x) \in \mathbb{C} \quad \text{"wave function"}$$

whose physical interpretation is: $|\psi(x)|^2 dx$ is the probability density for the presence of the particle. Hence we must have

$$\int_{\mathbb{R}^3} |\psi(x)|^2 dx = 1 = \|\psi\|_2^2$$

(and of course changing the value of $\psi(x)$ on a set of Lebesgue measure zero does not change the probability measure) so

$$\psi \in L^2(\mathbb{R}^3, \mathbb{C})$$

Remark: A phase $e^{i\alpha}$ does not change the state.

- The Hamiltonian function must be replaced by the energy functional

$$E(\psi) = T(\psi) + V(\psi) \quad \text{where}$$

$$T(\psi) = \frac{\hbar^2}{2m} \int_{\mathbb{R}^3} |\nabla\psi(x)|^2 dx$$

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

$\hbar$: Planck's constant

Rephrasing the stability of matter problem: is

$$E_0 := \inf \{ E(\psi) : \psi \in L^2(\mathbb{R}^3; \mathbb{C}),\ \|\psi\|_2 = 1 \}$$

finite? $\rightsquigarrow$ Calculus of variations

4)

More specific question: if $E_0 > -\infty$, is the infimum a minimum, namely is there a (unique?) ground state Ψ_0 s.t.

$$E_0 = E(\Psi_0)$$

Classically: the positive T could not compensate the negative V

Quantum mechanically T and V are not independent

⇝ "Uncertainty principles"

1) Heisenberg: For any $\|\Psi\|_2 = 1$:

$$\int |\nabla\Psi(x)|^2 dx \geq C \left(\int |\Psi(x)|^2 x^2 dx \right)^{-1}$$

i.e. if the particle is well localized close to $x=0$ then its kinetic energy must be very large.

2) A more useful one: Gagliardo-Nirenberg-Sobolev.

If Ψ vanishes at infinity, i.e.

$|\{x : \Psi(x) > a\}| < \infty$ for all $a > 0$,

and if $\nabla\Psi \in L^2$, then

$$\|\Psi\|_6^2 \leq C \|\nabla\Psi\|_2^2 , \quad C^{-1} = \frac{3}{4}(4\pi^2)^{2/3}$$

Sobolev conjugate of 2: $\frac{1}{p^*} = \frac{1}{p} - \frac{1}{d} = \frac{1}{2} - \frac{1}{3}$

namely $\underbrace{\int_{\mathbb{R}^3} |\nabla\Psi(x)|^2 dx}_{= 2T(\Psi)} \geq \frac{3}{4}(4\pi^2)^{2/3} \underbrace{\left(\int |\Psi(x)|^6 dx \right)^{1/3}}_{\text{relate to } V(\Psi)}$

⇝ Proof of stability (of the first kind)

Hölder's inequality: for any $1 \leq p, q \leq \infty$ s.t. $p^{-1} + q^{-1} = 1$

$$\int \overline{f(x)}\, g(x)\, dx \leq \|f\|_p \|g\|_q$$

provided $f \in L^p$, $g \in L^q$

So: if $V \in L^{3/2}(\mathbb{R}^3)$

$$|V(\psi)| \leq \int |\psi(x)|^2 |V(x)|\, dx$$

$$\leq \underbrace{\| |\psi|^2 \|_3}_{= \left(\int |\psi(x)|^6\right)^{1/3}} \| |V| \|_{3/2} \qquad \left(\frac{1}{3} + \frac{2}{3} = 1\right)$$

Hence with (2)

$$2T(\psi) \geq \frac{3}{4}(4\pi^2)^{2/3} \frac{1}{\|V\|_{3/2}} |V(\psi)| ,$$

and so

$$T(\psi) + V(\psi) \geq \left(\frac{3}{8} \frac{(4\pi^2)^{2/3}}{\|V\|_{3/2}} - 1 \right) |V(\psi)|$$

Conclusion!

$$E(\psi) \geq 0 \quad \text{for all } \psi \in L^2 : \nabla\psi \in L^2 ,$$

provided $\|V\|_{3/2} \leq \frac{3}{8}(4\pi^2)^{2/3}$.

- Note that the Coulomb potential is not in the right space: $\frac{1}{|x|^{3/2}}$ is integrable at 0, but it is not at ∞. so we need a bit more gymnastics.

If $V(x) = V_1(x) + V_2(x)$

$V_1 \in L^{3/2}(\mathbb{R}^3)$, $V_2 \in L^\infty(\mathbb{R}^3)$ (i.e. bounded)

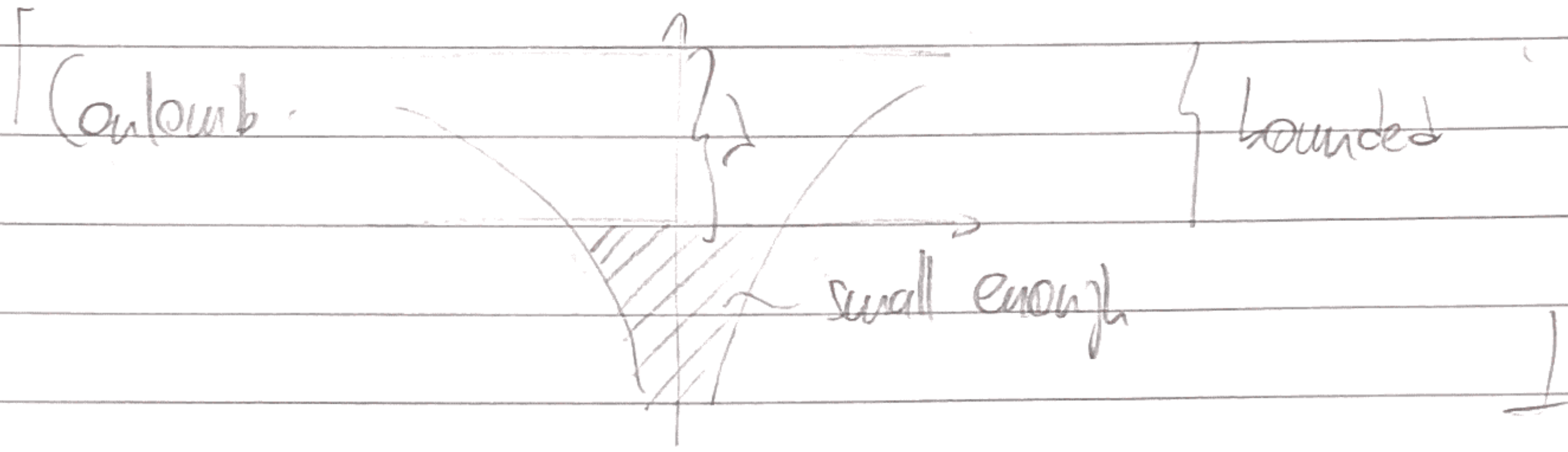
6)

Pick $\lambda \in \mathbb{R}$ s.t.

$$v(x) = \min\left(V_1(x) - \lambda, 0\right)$$

is such that

$$\|v\|_{3/2} \leq \frac{1}{2}\frac{3}{8}\left(4\pi^2\right)^{2/3}$$



then $v(\psi) \geq \frac{1}{2} T(\psi)$ a ! so

$$T(\psi) + V(\psi) = T(\psi) + \left(V_1(\psi) - \lambda\right) + \lambda + V_2(\psi)$$
$$\geq \frac{1}{2} T(\psi) + \lambda - \|V_2\|_\infty$$

since $\int |V_2(x)||\psi(x)|^2 dx \leq \sup_x |V_2(x)| \overbrace{\int |\psi(x)|^2 dx}^{=1}$

so that $\lambda - \|V_2\|_\infty$ is a lower bound for E

Note: The power of the method lies in its generality. Stability is not specific to the hydrogen atom $V(x) \propto 1/|x|$, which can be seen by elementary methods.

- In the specific case of the hydrogen atom

$$E(\psi) = \int \left(\frac{1}{2}|\nabla\psi(x)|^2 - \frac{\alpha}{|x|}|\psi(x)|^2\right) dx$$

the minimizer is explicit

$$\psi_0 = C e^{-\alpha|x|}$$

and

$$E_0 = E(\psi_0) = -\frac{\alpha^2}{2}$$

2 Structure of quantum mechanics

- State space : Hilbert space $\mathcal{H}$
  a complete inner product space. Notation
  $\langle \psi, \varphi \rangle$ and $\langle \psi, \psi \rangle = \|\psi\|^2$ (*)

Examples: * $\mathcal{H} = L^2(\mathbb{R}^3)$, $\langle \psi, \varphi \rangle = \int \bar{\psi}(x) \varphi(x) dx$
* $\mathcal{H} = \ell^2(\mathbb{N})$, $\langle \psi, \varphi \rangle = \sum_{i=1}^{\infty} \bar{\psi}_i \varphi_i$
* $\mathcal{H} = \mathbb{C}^N$, $\langle \psi, \varphi \rangle = \sum_{i=1}^{N} \bar{\psi}_i \varphi_i$

- Dirac notation : $\psi \in \mathcal{H}$ denoted $|\psi\rangle$.
  Then $|\psi\rangle\langle\psi|$ represents the projection onto the ray of ψ :

$$(|\psi\rangle\langle\psi|)|\varphi\rangle = \langle\psi|\varphi\rangle|\psi\rangle$$

- A useful Lemma : polarization identity

$$\langle \psi, \varphi \rangle = \frac{1}{4}\left(\|\psi+\varphi\|^2 - \|\psi-\varphi\|^2 + i\|\psi - i\varphi\|^2 - i\|\psi + i\varphi\|^2 \right)$$

  i.e. the inner product is completely determined by the norm in a complex Hilbert space.
- In this course : $\mathcal{H}$ is separable : there exists a countable orthonormal basis, and every ON basis is countable

(*) $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ st
  (i) linearity : $\langle \psi, \alpha_1 \varphi_1 + \varphi_2 \rangle = \alpha_1 \langle \psi, \varphi_1 \rangle + \langle \psi, \varphi_2 \rangle$
  (ii) antisymmetry : $\langle \varphi, \psi \rangle = \overline{\langle \psi, \varphi \rangle}$
  (iii) positive definite : $\langle \psi, \psi \rangle \geq 0$ and $= 0 \Leftrightarrow \psi = 0$.

* Cauchy-Schwartz inequality

$$|\langle \psi, \varphi \rangle| \leq \|\psi\| \, \|\varphi\|$$

* Consequence: triangle inequality:

$$\|\psi + \varphi\| \leq \|\psi\| + \|\varphi\|$$

8)

- Physical observables are represented by self-adjoint linear operators on $\mathcal{H}$
Example: $\mathcal{H} = L^2(\mathbb{R})$
Observable P_Ω: Is the particle in the subset $\Omega \subset \mathbb{R}$?

$$(P_\Omega \psi)(x) = \chi_\Omega(x)\psi(x)$$

$\uparrow$ characteristic function of Ω

Note $P_\Omega = P_\Omega^\dagger = P_\Omega^2$ "orthogonal projection"

* Expectation value of P_Ω in state ψ:

$$\langle \psi, P_\Omega \psi \rangle = \int_\Omega |\psi(x)|^2 dx$$

is the probability that the particle is in Ω.

* Eigenvalues of P_Ω: 0, 1 are the possible results of a measurement

* For the corresponding eigenvectors $P_\Omega v = \lambda v$, the result of the measurement is "deterministic":
$\langle v, P_\Omega v \rangle = \lambda \|v\|^2 = 0$ or 1

Another observable: position operator X
$(X\psi)(x) = x\psi(x)$ $\qquad \langle X \rangle_\psi$
(multiplication operator)
Expectation value: $\langle \psi, X\psi \rangle = \int x |\psi(x)|^2 dx$
Variance:

$$\langle (\Delta X)^2 \rangle_\psi = \int (x - \langle x \rangle_\psi)^2 |\psi(x)|^2 dx$$

$$= \|(x - \langle x \rangle_\psi)\psi\|^2 \geq 0$$

Note: For a general operator A
if $A\psi = \lambda\psi$, then $\langle (\Delta A)^2 \rangle_\psi = 0$
$\rightsquigarrow$ see later definition of spectrum

- More on linear operators

range of A

$$A : \mathcal{D}(A) \to \mathcal{R}(A) \subset \mathcal{H}$$

domain of A, always assumed to be dense

If $\psi \in \mathcal{D}(A)$ then $A\psi \in \mathcal{H}$

A is linear: $A(\alpha\psi_1 + \psi_2) = \alpha A\psi_1 + A\psi_2$

A is bounded if

$$\|A\psi\| \leq C\|\psi\|$$

with C independent of ψ. $A \in \mathcal{L}(\mathcal{H})$

The smallest such C is defined to be $\|A\|$.

$$\|A\| := \sup\left\{ \frac{\|A\psi\|}{\|\psi\|} : \psi \in \mathcal{H},\ \psi \neq 0 \right\}$$

least upper bound.

If the supremum $= +\infty$ then A is unbounded

Rules:
- $A = B$ if $\mathcal{D}(A) = \mathcal{D}(B)$ and $A\psi = B\psi$ $\forall \psi \in \mathcal{D}(A)$
- $A \subset B$ if $\mathcal{D}(A) \subset \mathcal{D}(B)$ and ——"——
  B is an extension of A
- $\mathcal{D}(A+B) = \mathcal{D}(A) \cap \mathcal{D}(B)$ (and there may be extensions)
- $\mathcal{D}(AB) = \{\psi \in \mathcal{D}(B) : B\psi \in \mathcal{D}(A)\}$ "
- Inverse exists if A is injective (one-to-one)
  $\mathcal{D}(A^{-1}) = \mathcal{R}(A)$, $\mathcal{R}(A^{-1}) = \mathcal{D}(A)$

A criterion for injectivity:

$$A \text{ injective} \Leftrightarrow \mathrm{Ker}(A) = \{0\}$$

" $\{\psi \in \mathcal{D}(A) : A\psi = 0\}$

Ker$(z-A) = \{0\}$; $R(z-A) = \mathcal{H}$ and $(z-A)^{-1}$ is bounded.

- Resolvent set of A:
$$\rho(A) = \{z \in \mathbb{C} : (z-A)^{-1} \text{ exists and is bounded}\}$$
resolvent of A at z.

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

Lemma: $\sigma(A)$ is closed, $\rho(A)$ is open (in $\mathbb{C}$)

Resolvent identity:
$$(z-A)^{-1} - (w-A)^{-1} = (w-z)(z-A)^{-1}(w-A)^{-1}$$
for any $z, w \in \rho(A)$

$\leadsto$ in particular: $(z-A)^{-1}$ commutes with $(w-A)^{-1}$

If $z-A$ has a non-trivial kernel, i.e. $\exists \psi \neq 0$ s.t. $A\psi = z\psi$, then $z-A$ is not injective and hence $z \in \sigma(A)$.
The vector ψ is called an eigenvector and z is an eigenvalue.

Note: Not all $z \in \sigma(A)$ are eigenvalues.

Ex: Multiplication operator
$$(A\psi)(x) = f(x)\psi(x)$$
(f: any measurable function)

$(A-z)^{-1}$ is a multiplication operator
$$((A-z)^{-1}\psi)(x) = \frac{1}{f(x)-z}\psi(x)$$
with
$$\mathcal{D}((A-z)^{-1}) = \left\{\psi : \frac{\psi(x)}{f(x)-z} \in L^2(\mathbb{R})\right\}$$

Now: $$\left\|\frac{\psi(\cdot)}{f(\cdot)-z}\right\|_2 \leq \left\|\frac{1}{f(\cdot)-z}\right\|_\infty \|\psi\|_2$$

So that $$\|(A-z)^{-1}\| = \left\|\frac{1}{f(\cdot)-z}\right\|_\infty.$$

When is this bounded? If $\exists \varepsilon > 0$ s.t.
$$|\{x \in \mathbb{R} : f(x) - z < \varepsilon\}| = 0$$

Hence $\rho(A) = \{z : \exists \varepsilon > 0 : |\{x : |f(x) - z| < \varepsilon\}| = 0\}$.

and so

Theorem: $\sigma(A) = \{z : \forall \varepsilon > 0 : |\{x : |f(x) - z| < \varepsilon\}| > 0\}$.

"essential range of f"

If f is continuous: $\sigma(A) = \overline{\text{range of } f}$.

For example: Position operator:

$$\sigma(X) = \mathbb{R}$$

Are there eigenvalues? Solutions of $f(x)\psi(x) = z\psi(x)$ for almost all $x \in \mathbb{R}$

For all x s.t. $f(x) \neq z$, we must have $\psi(x) = 0$

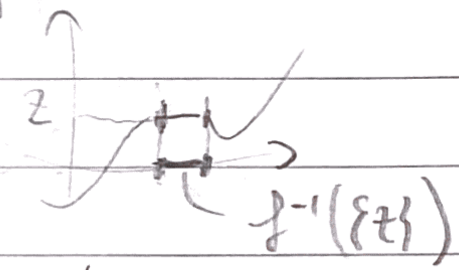
Hence $\psi = 0$ if $|\{x : f(x) = z\}| = 0$

i.e. $\operatorname{Ker}(z - A) = 0$ if $|f^{-1}(\{z\})| = 0$

and

z is an eigenvalue $\Leftrightarrow$ $|f^{-1}(\{z\})| > 0$

"flat part of f"



In particular: the position operator X (multiplication by $f(x) = x$) has no eigenvalue but P_Ω (multiplication by $f(x) = \chi_\Omega(x)$) has eigenvalues $\{0, 1\}$

- Let $A : D(A) \to \mathcal{H}$. The adjoint $A^\dagger$ of A is defined as follows:

$$\varphi \in D(A^\dagger) \Leftrightarrow |\langle \varphi, A\psi \rangle| \leq C\|\psi\| \quad \text{for all } \psi \in D(A)$$

In other words: the map

$$\psi \mapsto \langle \varphi, A\psi \rangle$$

is a bounded linear map. By Riesz' lemma (see later), there is a unique $\xi \in \mathcal{H}$ s.t.

$$\langle \varphi, A\psi \rangle = \langle \xi, \psi \rangle$$

and we define $A^\dagger$ on $D(A^\dagger)$ by $\xi = A^\dagger \varphi$.
Equivalently:

$$\langle \varphi, A\psi \rangle = \langle A^\dagger \varphi, \psi \rangle \qquad (\forall \psi \in D(A),\ \varphi \in D(A^\dagger))$$

The subtlety here is that $D(A)$ is in general different from $D(A^\dagger)$

Check: If A is bounded:
- $\|A^\dagger\| = \|A\|$
- $(\lambda A)^\dagger = \bar{\lambda} A^\dagger$
- $(A+B)^\dagger = A^\dagger + B^\dagger$
- $(AB)^\dagger = B^\dagger A^\dagger$
- $A^{\dagger\dagger} = A$

Definition: (i) A is symmetric if

$$\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle \qquad \forall \varphi, \psi \in D(A)$$

(ii) A is self-adjoint if $A = A^\dagger$

Notes: * Symmetric $\Leftrightarrow$ $A \subset A^\dagger$ $\left(|\langle \varphi, A\psi \rangle| \leq \|A\varphi\| \|\psi\| \text{ so } \psi \mapsto \langle \varphi, A\psi \rangle \text{ is bounded for each } \varphi \in D(A) \right)$
* If A, B are bounded and defined on all of $\mathcal{H}$ (this can always be done), then symmetric $\Leftrightarrow$ self-adjoint (in particular if $\dim \mathcal{H} < \infty$)

$\rightsquigarrow$ examples later.

- Spectral theorem. Let $A = A^\dagger$. There is a unique map $f \mapsto f(A)$ such that

* $(\alpha f + g)(A) = \alpha f(A) + g(A)$ (i)
* $(fg)(A) = f(A) g(A)$ (ii)
* $\bar{f}(A) = f(A)^*$ (iii)
* $f(A) = \begin{cases} \mathbb{1} & \text{for } f(x) = 1 \\ A & \text{for } f(x) = x \end{cases}$ (iv)

Here: f is a Borel function. This set $\mathcal{B}(\mathbb{R})$ is the smallest set of functions that contains all continuous functions vanishing at $\pm\infty$ and that is closed under pointwise convergence: $f_n \in \mathcal{B}(\mathbb{R})$ and $f_n(x) \to f(x)\ \forall x$ implies $f \in \mathcal{B}(\mathbb{R})$

For finite dimensional matrices: $A = \sum_j a_j |\varphi_j\rangle\langle\varphi_j|$ and

$$f(A) = \sum_j f(a_j)\, |\varphi_j\rangle\langle\varphi_j|$$

for example: exponential of a matrix.

- Now for any interval $I \subset \mathbb{R}$:

$$P_I(A) = \chi_I(A) \quad \text{is an orthogonal projection.}$$

$$P_I(A) = P_I(A)^2 = P_I(A)^* \quad \text{(by (ii, iii) above)}$$

and if $I_1 \cap I_2 = \emptyset$

$$P_{I_1}(A) + P_{I_2}(A) = P_{I_1 \cup I_2}(A) \quad \text{(by (i))}$$

(and countably so)

Hence: for any $\psi \in \mathcal{H}$:

$$\mu_\psi^A(I) = \langle \psi, P_I(A)\psi \rangle \quad \text{"spectral measure"}$$

is a probability measure on $\mathbb{R}$:

- $\mu_\psi^A(I) = \|P_I(A)\psi\|^2 \geq 0$
- Additivity: $\mu_\psi^A(I_1) + \mu_\psi^A(I_2) = \mu_\psi^A(I_1 \cup I_2)$ $(I_1 \cap I_2 = \emptyset)$
- $\mu_\psi^A(\mathbb{R}) = 1$

Physical interpretation: $\mu_\psi^A(I)$ is the probability that a measurement of A returns a value $x \in I$ if the system was in state ψ just before the measurement.

We recover (a little bit sloppy) the expectation value introduced above.
Probability of measurement in $(\lambda, \lambda + d\lambda]$ is $d\mu_\psi^A((-\infty, \lambda])$ and so the expectation value is

$$\langle A \rangle_\psi = \int \lambda \, d\mu_\psi^A((-\infty, \lambda])$$

$$= \int \lambda \, d\langle \psi, P_{(-\infty,\lambda]}(A)\psi \rangle$$

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

Since
$$\int \lambda \, d\chi_{(-\infty,\lambda]}(x) = x$$
and (iv) above.

$\rightsquigarrow$ Note one writes

$$A = \int \lambda \, dP_\lambda$$

and it is analogous to $A = \sum_j a_j |\varphi_j\rangle\langle\varphi_j|$ in the case $\dim \mathcal{H} < \infty$.

- Variance: $\langle (\Delta A)^2 \rangle_\psi := \langle (A - \langle A \rangle_\psi)^2 \rangle_\psi$

$$= \| (A - \langle A \rangle_\psi)\psi \|^2 = \langle A^2 \rangle_\psi - \langle A \rangle_\psi^2$$

from here. $\langle (\Delta A)^2 \rangle_\psi = 0$

$$\Leftrightarrow A\psi = \langle A \rangle_\psi \psi$$

namely: the variance in the measurement outco vanishes iff ψ is an eigenstate of A

Remarks: * If $\sigma(A)$ is made up of non-degenerate eigenvalues only, then

$$P_I(A) = \sum_{a \in \sigma(A) \cap I} |\varphi_a\rangle\langle\varphi_a|$$

⇝ Probability of measurement $a \in \mathbb{R}$: $\langle \psi, P_a \psi \rangle$, namely

$$|\langle \varphi_a, \psi \rangle|^2$$

In particular: if $\psi = \varphi_b$

$$\text{Prob}(\text{measurement} = a) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise,} \end{cases}$$

(compare with variance!)

* Repeating a measurement just after the measurement should yield the same result
⟹ The state of the system immediately after the measurement with result a is φ_a
⇝ "collapse" of the wave function.

• Proposition [Heisenberg] For A, B bounded, self-adjoint

$$\langle (\Delta A)^2 \rangle_\psi \langle (\Delta B)^2 \rangle_\psi \geq \frac{1}{4} |\langle [A,B] \rangle_\psi|^2$$

Proof: $|\langle \psi, [A,B]\psi \rangle| = |\langle A\psi, B\psi \rangle - \langle B\psi, A\psi \rangle|$

$$\leq 2 \|A\psi\| \|B\psi\|$$

The claim follows by taking the square and replacing $A \to A - \langle A \rangle_\psi$, $B \to B - \langle B \rangle_\psi$ (and $[A,B] \to [A,B]$.) □

16)

Indeed: Two non-commuting operators do not in general have common eigenvectors hence they cannot both have sharply defined values

- Return to Riesz' lemma.

* For any $\varphi \in \mathcal{H}$, the map $l_\varphi : \mathcal{H} \to \mathbb{C}$ given by $l_\varphi(\psi) = \langle \varphi, \psi \rangle$ is a bounded linear functional:
$$|l_\varphi(\psi)| \leq \|\varphi\| \|\psi\| \qquad (\text{norm } \|\varphi\|)$$
* Riesz' lemma claims that all bounded linear functionals arise in this way:
Let l be a bdd linear functional on $\mathcal{H}$. There is a unique $\eta_l \in \mathcal{H}$ s.t. $l(\psi) = \langle \eta_l, \psi \rangle$ for all $\psi \in \mathcal{H}$.

Proof: $\mathcal{N} := \{\psi \in \mathcal{H} : l(\psi) = 0\} = l^{-1}(\{0\})$ is closed since l is continuous (because bdd). If $\mathcal{N} = \mathcal{H}$, we pick $\eta_l = 0 \in \mathcal{H}$. Otherwise $\exists\ \eta \in \mathcal{N}^\perp$ (i.e. $\langle \eta, \psi \rangle = 0\ \forall \psi \in \mathcal{N}$) with $\|\eta\| = 1$. For any $\psi \in \mathcal{H}$,
$$l\big(l(\psi)\eta - l(\eta)\psi\big) = 0 \quad (\text{by linearity})$$
So that $l(\psi)\eta - l(\eta)\psi \in \mathcal{N}$ and
$$0 = \langle \eta, l(\psi)\eta - l(\eta)\psi \rangle = l(\psi) - l(\eta)\langle \eta, \psi \rangle$$
$$\Rightarrow \langle \eta, \psi \rangle = \frac{l(\psi)}{l(\eta)} \quad \text{namely}$$
$\eta_l := \overline{l(\eta)} \cdot \eta$ has the right properties.

Uniqueness
$$\langle \eta_l' - \eta_l, \psi \rangle = l(\psi) - l(\psi) = 0 \quad \forall \psi \in \mathcal{H}$$
$\Rightarrow \eta_l' - \eta_l \in \mathcal{H}^\perp$, namely $\eta_l' - \eta_l = 0$ $\square$

- **Corollary**: Let $b(\varphi,\psi)$ be a sesquilinear form on $\mathcal{H}\times\mathcal{H}$

  $b : \mathcal{H}\times\mathcal{H}\to\mathbb{C}$: b is $\begin{cases}\text{linear in } \psi \\ \text{antilinear in } \varphi\end{cases}$

  If b is bounded:

  $$|b(\varphi,\psi)| \leq C\,\|\varphi\|\,\|\psi\|$$

  Then there is a unique bounded operator B on $\mathcal{H}$ s.t.

  $$b(\varphi,\psi) = \langle \varphi, B\psi\rangle$$

- The momentum operator in QM P on $\mathcal{H} = L^2([0,1])$

  * Derivative of $\psi\in\mathcal{H}$ understood in the sense of distributions

  $$\psi' : C_c^\infty([0,1]) \to \mathbb{C}$$
  $$v \mapsto \psi'[v] = -\int_0^1 \psi(x)\,v'(x)\,dx$$

  (formal int by parts)

  * Lemma [Morrey]

  If $\psi'\in L^2([0,1])$, then ψ is continuous, and for any φ s.t. $\varphi'\in L^2([0,1])$:

  $$\int_0^1 \big(\psi'(x)\varphi(x) + \psi(x)\varphi'(x)\big)\,dx = \psi(x)\varphi(x)\Big]_0^1$$

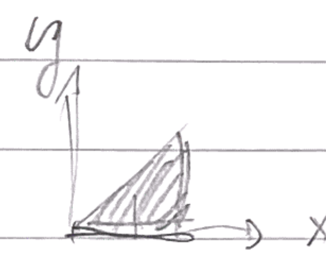
  Idea of proof: Define $\tilde{\psi}(x) = \int_0^x \psi'(y)\,dy$.

  ◇ Well-defined by Cauchy-Schwarz

  $$\int_0^x |\psi'(y)|\,dy \leq \left(\int_0^x |\psi'(y)|^2\,dy\right)^{1/2}\left(\int_0^x 1\right)^{1/2}$$

  ◇ Continuous (as the int. of a measurable function)

  ◇ $\psi' = \tilde{\psi}'$. Indeed:

  $$\tilde{\psi}'[v] = -\int_0^1 \tilde{\psi}(x)\,v'(x)\,dx$$

  the L^2 function

  $$= -\int_0^1 v'(x)\int_0^x \psi'(y)\,dy\,dx$$

  $$= -\int_0^1\int_y^1 v'(x)\,\psi'(y)\,dx\,dy$$

  $$= -\int_0^1 \psi'(y)\big(\underbrace{v(1)}_{=0} - v(y)\big)\,dy$$

$= \int_0^1 \psi'(y) v(y) dy = \psi'[v]$

Finally $\tilde{\psi}'[v] - \psi'(v) = 0 \quad \forall v \Rightarrow \psi = \text{constant}$ $\square$

Define. (i) $D(\tilde{P}) = \{\psi \in \mathcal{H} : \psi' \in \mathcal{H}\}$; $\tilde{P}\psi = -i\psi'$

(ii) $D(P_0) = \{\psi \in D(\tilde{P}) : \psi(0) = \psi(1) = 0\}$; $P_0\psi = \tilde{P}\psi$

(well-defined by lemma)

Clearly : $P_0 \subsetneq \tilde{P}$

Claim : $P_0 = \tilde{P}^*$

Proof : $\varphi \in D(\tilde{P}^*)$ iff $|\langle \varphi, \tilde{P}\psi \rangle| \le C\|\psi\|$ for all $\psi \in D(\tilde{P})$

In particular (by picking $\psi = v \in C_c^\infty([0,1])$)

$|\varphi'[v]| \le C\|v\|$

So φ defines a bdd lin. functional on the dense set $C_c^\infty([0,1])$. By Riesz Lemma:

$\varphi' \in L^2([0,1])$, namely $\varphi \in D(\tilde{P})$

proved: $D(\tilde{P}^*) \subset D(\tilde{P})$

it remains to show: $\varphi(0) = \varphi(1) = 0$

Now for any $\psi \in D(\tilde{P})$

$(*) \quad \langle \tilde{P}\psi, \varphi \rangle - \langle \psi, \tilde{P}\varphi \rangle = i \int_0^1 (\bar{\psi}'\varphi - \bar{\psi}\varphi')$

$= i(\bar{\psi}(1)\varphi(1) - \psi(0)\varphi(0))$

by the lemma ; We note:

$|\langle \psi, \tilde{P}\varphi \rangle| / \|\psi\| \le \|\tilde{P}\varphi\|$

but the r.h.s. can be made arbitrarily big by concentrating ψ at 1 or 0. Hence

$|\langle \tilde{P}\psi, \varphi \rangle| / \|\psi\|$

is bounded for all ψ iff $\varphi(0) = \varphi(1) = 0$

namely: $\varphi \in D(\tilde{P}^*)$

$\Rightarrow D(\tilde{P}^*) = D(P_0)$

and $\tilde{P}^*\varphi = \tilde{P}\varphi = P_0\varphi$

Note : For $\varphi, \psi \in D(P_0)$ $(*) \Rightarrow \langle \tilde{P}\psi, \varphi \rangle = \langle \psi, \tilde{P}\varphi \rangle$

namely :

P_0 is symmetric

but not self-adjoint : $P_0 \subsetneq \tilde{P} = \tilde{P}^{**} = P_0^*$
$\tilde{P}$ closed

Question : can we extend P_0 (namely find a domain between $\mathcal{D}(P_0)$ and $\mathcal{D}(\tilde{P})$) so that $-i\frac{d}{dx}$ becomes self-adjoint ?

Answer: yes, there is a 1-parameter family of s.-a. extensions.

For $\alpha \in \mathbb{C}$, $|\alpha| = 1$, define

$$\mathcal{D}(P_\alpha) := \{\psi \in \mathcal{D}(\tilde{P}) : \psi(1) = \alpha\psi(0)\}$$
$$P_\alpha\psi = \tilde{P}\psi$$

Clearly : $P_0 \subset P_\alpha \subset \tilde{P}$

Claim : $P_\alpha = P_\alpha^*$

As above : First : $\mathcal{D}(P_\alpha^*) \subset \mathcal{D}(\tilde{P})$
Second : For $\psi \in \mathcal{D}(P_\alpha)$:

$$\langle \tilde{P}\psi, \varphi\rangle - \langle \psi, \tilde{P}\varphi\rangle = i\bar{\psi}(0)\left(\bar{\alpha}\varphi(1) - \varphi(0)\right)$$

and by the same reasoning :
$\varphi \in \mathcal{D}(P_\alpha^*)$ iff $\varphi(1) - \alpha\varphi(0) = 0$ namely $\varphi \in \mathcal{D}(P_\alpha)$

Summary : * All P's above act as $-i\frac{d}{dx}$.
* With Dirichlet b.c. P_0 is symmetric, not self-adjoint
* With periodic b.c. (and a magnetic flux) : P_α is self-adjoint
* P_0 and P_α differ non-trivially despite agreeing on a dense set $\mathcal{D}(P_0)$.
Example ($\alpha = 1$) : P_0 has no eigenvector but P_1 has a ON basis of eigenvectors:
$$\varphi_n(x) = e^{2\pi i n x}$$
* Self-adjointness is crucial for a physical dynamics ⤳ see later (Stone's theorem)

In fact: As a differential equation, the eigenvalue eq
$$-i\psi' = z\psi$$
has a unique solution $\psi(x) = e^{izx} \cdot C$ for all $z \in$

i) $\tilde{P}$: For any $z \in \mathbb{C}$: $Ce^{izx} \in L^2([0,1])$ and
$\psi' = ize^{izx} \in L^2([0,1]) \rightsquigarrow$ all $z \in \mathbb{C}$ are eigenvalu
$\sigma(\tilde{P}) = \mathbb{C}$

ii) P_α : $\psi(1) = \alpha\psi(0) \Leftrightarrow e^{iz} = \alpha$
namely $z = \log_{[0,2\pi]}(\alpha) + 2\pi n,\ n \in \mathbb{Z}$

iii) P_0 : $\psi(1) = 0,\ \psi(0) = 0 \rightsquigarrow C = 0$
$\Rightarrow$ no eigenvector

- We have seen:
  (i) Symmetric operators may have many self-adjoint extensions
  (ii) Physics often comes with a formal "quadratic form" for the energy (Hamiltonian) which is bounded below. Example (simplest)
$$E(\psi) = \int |\nabla\psi(x)|^2 dx \geq 0$$
$\rightsquigarrow$ Q: Is there a natural self-adjoint operator associ with a bounded quadratic form?
A: Yes: "Friedrich's extension"

As an example: Consider $T = -\frac{d^2}{dx^2}$ defined on $C_c^\infty((0,1))$ which is dense in $L^2((0,1))$

* $\langle\psi, T\psi\rangle = -\int_0^1 \overline{\psi(x)}\,\psi''(x)\,dx$
$$\overset{\text{IBP}}{=} \int_0^1 \overline{\psi(x)'}\,\psi(x)'\,dx = \int_0^1 |\psi'(x)|^2 dx \geq 0$$

* In general: A densely defined operator is called nonnegative if the associated quadratic form
$$q_T(\psi) = \langle\psi, T\psi\rangle \geq 0 \quad \forall \psi \in D(T)$$

- **Lemma** $\langle \psi, T\psi \rangle \in \mathbb{R}$ for all $\mathcal{D}(T)$
  $\Leftrightarrow$ T is symmetric.

In other words:
the fact that expectation value are real "only" yields that T is symmetric not self-adjoint.

Proof: + T symmetric
$$\Rightarrow \langle \psi, T\psi \rangle = \langle T\psi, \psi \rangle = \overline{\langle \psi, T\psi \rangle}$$
so $\langle \psi, T\psi \rangle \in \mathbb{R}$

+ Reciprocally: Let $\varphi, \psi \in \mathcal{D}(T)$. Then we have the polarization identity:
$$\langle \varphi, T\psi \rangle = \frac{1}{4}\Big[\langle \varphi+\psi, T(\varphi+\psi) \rangle - \langle \varphi-\psi, T(\varphi-\psi) \rangle$$
$$- i\langle \varphi+i\psi, T(\varphi+i\psi) \rangle + i\langle \varphi-i\psi, T(\varphi-i\psi) \rangle \Big]$$
and all inner products on the RHS are real.
Now, $\langle T\varphi, \psi \rangle = \overline{\langle \psi, T\varphi \rangle}$ is obtained from the above by (i) exchanging $\psi \leftrightarrow \varphi$
(ii) taking the conjugate
Both terms in the first line are invariant under (i,ii) while the two terms on the second line are exchanged
Hence $\langle T\varphi, \psi \rangle = \langle \varphi, T\psi \rangle$ indeed ☒

- Strategy of the construction of the Friedrichs extension of a positive operator $T \geq 0$
Note: if $T \geq \gamma$ the strategy applies to $T - \gamma$.
(i) Define quadratic form
$$q_T(\psi) = \langle \psi, T\psi \rangle \geq 0$$
on $\mathcal{D}(T)$. By polarization, we also have $q_T(\varphi, \psi)$.
Because T is positive,
$$\langle \varphi, \psi \rangle_T := \langle \varphi, T\psi \rangle + \langle \varphi, \psi \rangle$$
defines an inner product on $\mathcal{D}(T)$
(ii) Consider the completion $\underbrace{\text{of } \mathcal{D}(T)}_{Q(T)}$ w.r.t. $\|\cdot\|_T$

and embed $Q(T)$ in $\mathcal{H}$ (technicalities are here)

(iii) Extend q_T on $\mathcal{D}(T)$ to $\hat{q}_T$ on $Q(T)$. This ensures that $\hat{q}_T$ is closed:
if $\psi_n \in Q(T)$, $\psi_n \to \psi$ in $\mathcal{H}$, $\hat{q}_T(\psi_n - \psi_m) \to 0$
then $\psi \in Q(T)$ and $\hat{q}_T(\psi_n - \psi, \psi_n - \psi) \to 0$.

(iv) By a version of Riesz' lemma, define

$$\langle \varphi, \hat{T}\psi \rangle = \hat{q}_T(\varphi, \psi)$$

and show that it is self-adjoint on a domain $\mathcal{D}(\hat{T}) \subset Q(T)$ (more technicalities here)

We obtain

- **Theorem**: Let $T \geq 0$. There is a unique self-adjoint operator $\hat{T}$ s.t.
  (i) $T \subset \hat{T}$ ($\hat{T}$ is an extension of T)
  (ii) $\hat{T} \geq 0$
  (iii) $\mathcal{D}(\hat{T}) \subset Q(T)$.

- Examples: $\times$ $T = -\dfrac{d^2}{dx^2}$ on $C_c^\infty((0,1)) = \mathcal{D}(T) \subset L^2([0,1])$

$$\langle \psi, T\psi \rangle = \int_0^1 |\psi'(x)|^2 dx \geq 0$$

by integration by parts.

The inner product induced by T yields the norm

$$\|\psi\|_T^2 = \langle \psi, T\psi \rangle + \langle \psi, \psi \rangle = \|\psi'\|_2^2 + \|\psi\|_2^2$$

In particular: $\psi \in Q(T) \Rightarrow \psi' \in L^2$ and hence ψ is continuous.

Moreover: if $\psi_n \to \psi$ w.r.t. $\|\cdot\|_T$,

$$|\psi_n(x) - \psi(x)| \leq \int_0^x |\psi_n'(y) - \psi'(y)|\, dy \leq \|\psi_n' - \psi'\|_2$$

by Cauchy-Schwarz; hence $\psi_n \to \psi$ pointwise.
Since $\mathcal{D}(\tilde{T})$ is obtained as limits, in $\|\cdot\|_T$, of functions that are equal to zero at 0, 1, and the limit is pointwise:

If $\psi \in \mathcal{D}(\tilde{T})$, then
(i) $\psi' \in L^2([0,1])$
(ii) $\psi(0) = 0 = \psi(1)$

$\Rightarrow$ The Friedrichs extension of T is $-\frac{d^2}{dx^2}$ with Dirichlet boundary conditions.

Spectrum of $\tilde{T}$? The PDE
$$-\psi''(x) = \lambda\psi(x)$$
has two independent solutions $\sin(\sqrt{\lambda}x)$; $\cos(\sqrt{\lambda}x)$. They are in L^2 for all $\lambda \in \mathbb{C}$, and so are their derivatives.
The boundary condition however selects
$$\{\lambda_n = (n\pi)^2;\ n \in \mathbb{N}\} \text{ and } \psi_n(x) = \sin(n\pi x)$$
which form an ONB of $L^2([0,1])$

Note: We observe that $\tilde{T} \geq \pi^2$ and so the same must be true for the original quadratic form, namely
$$\int_0^1 |\psi'(x)|^2\,dx \geq \pi^2 \int_0^1 |\psi(x)|^2\,dx$$
for all $\psi \in C_c^1((0,1))$; "Poincaré's inequality"

Remark: There are other self-adjoint extensions of T. For example with B.C
$$\psi'(0) = 0 = \psi'(1)$$

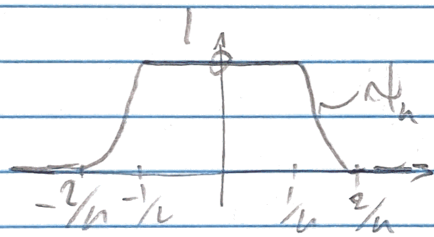
In that case, the constant function 1 is an eigenvector for eigenvalue 0, so this self-adjoint extension has a smaller lower bound than the original form.

* It is important that the form q_T arises from an operator. Consider

$$b(\varphi,\psi) = \overline{\varphi(0)}\psi(0)$$

Formally $b(\varphi,\psi) = \int \overline{\varphi(x)}\,\delta_0(x)\psi(x)\,dx$ but "the δ-function" is not an operator.

It turns out: $b(\varphi,\psi)$ is not closeable to a $\hat{b}$. Indeed:



$\psi_n \to 0$ in L^2

$b(\psi_n - \psi_m) = 0 \quad \forall n,m$

but

$b(\psi_n - 0) = 1, \ \forall n$