Introduction to Mathematical Physics: Quantum Dynamics, spring 2017

[Course information and announcemets from department's webpages (wiki.helsinki.fi/display/mathstatOpiskelu)]

1. Motivation & introduction

Double-slit experiment

* Modern version in the attached paper. (movies of the result available in a supplement: Direct links can be found from the course webpage.)

⇒ Single electrons going through a sufficiently closely spaced double-slit follow a probability distribution with a wave-like diffraction pattern!

[Solution: At small scales, Newtonian point particles are no longer an accurate description. Particles behave point-like only when "measured".]

⇒ Quantum mechanics

Newtonian (classical) particle:
complete description is trajectory in phase-space $(q(t), m\dot{q}(t))$, $q(t) \in \mathbb{R}^3$, $t \in \mathbb{R}$

Quantum particle:
complete description (when not measured) is wave-function $\psi(t) \in L^2(\mathbb{R}^3)$, $t \in \mathbb{R}$.

Measurement:
Q: Is particle in region $B \subset \mathbb{R}^3$ at time t?
A: With probability $\int_B dx\, |\psi(x,t)|^2$.

$\Rightarrow$ For consistency, <u>must</u> have

(1) $$\int_{\mathbb{R}^3} dx\, |\psi(x,t)|^2 = 1 \quad \forall t \in \mathbb{R}.$$

Schrödinger proposed that the wave-function of a free electron satisfies the PDE:

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = -\frac{\hbar^2}{2M} \Delta_x \psi(x,t) \;; \quad \Delta_x \psi = \sum_{i=1}^{3} \partial_{x_i}^2 \psi$$

$$\hbar = \frac{h}{2\pi} \approx 1{,}05 \cdot 10^{-34} \frac{m^2\, kg}{s},$$

$$M = m_e \approx 9{,}11 \cdot 10^{-31}\ kg.$$

From now on, we will use "units" $\hbar = 1 = m_e$, that is, we scale x and t suitably:

Let $\tilde{\psi}(\tilde{x}, \tilde{t}) = \psi(a\tilde{x}, b\tilde{t})$

$$a = 1\,\mathring{A} = 10^{-10} m, \quad b = a^2 \frac{M}{\hbar} \approx 8{,}68 \cdot 10^{-17} s.$$

Then $i\partial_{\tilde{t}} \tilde{\psi}(\tilde{x},\tilde{t}) = -\frac{1}{2}\Delta_{\tilde{x}} \tilde{\psi}(\tilde{x},\tilde{t})$, and we drop "~" in the following. Note that then
$\Delta\tilde{x} = 1 \Leftrightarrow \Delta x = 10^{-10} m$, $\Delta\tilde{t} = 1 \Leftrightarrow \Delta t \approx 10^{-16} s$.

Schrödinger also proposed that an electron in an external potential $V: \mathbb{R}^3 \to \mathbb{R}$ satisfies

$$(SE) \qquad i\partial_t \psi(x,t) = -\frac{1}{2}\Delta_x \psi(x,t) + V(x)\psi(x,t) .$$

For instance, the double slit experiment could then be treated by solving (SE) with some $\psi(x,0)$ (which takes into account the source) and using

$$V(x) = \begin{cases} \infty, & \text{if } x \in S = \{\text{Points inside slit}\} \\ 0, & \text{otherwise} \end{cases}$$

(or some smooth approximation of this, or B.C.)

[However, (1) <u>must</u> hold for all t !]

$\Rightarrow$ surprisingly subtle mathematical problem.

Outline of the solution:

- $L^2(\mathbb{R}^3)$ is a Hilbert space, with norm $\|\psi\|^2 = \int_{\mathbb{R}^3} dx\, |\psi(x)|^2$.
- Thus $(1) \Leftrightarrow \|\psi(t)\| = 1 \quad \forall t$
  $\Rightarrow \forall t \ \exists\, U(t): L^2 \to L^2$ s.t. $\psi(t) = U(t)(\psi(0))$ and $U(t)$ preserves norm.
- (SE) linear in ψ, assume $U(t)$ also linear
  $\Rightarrow U(t)$ unitary $\forall t$
- Consistency requires: $U(0) = 1$ and $U(t+s) = U(t)U(s) \quad \forall t, s \geq 0$.
- <u>Assume</u> continuity of the time-evol.

$\longrightarrow$

in the following precise sense:

$$\int_{\mathbb{R}^3} dx \; |\psi(x,t) - \psi(x,0)|^2 \xrightarrow{t \to 0} 0 .$$

then $U(t)$ is a "strongly continuous unitary semigroup".

$\Rightarrow \exists !$ "self-adjoint" operator H s.t.

$$U(t) = \text{"}e^{-itH}\text{"} \quad \forall t \in \mathbb{R}.$$

and $i \frac{d}{dt} \psi(t) = H \psi(t)$ for "many" $\psi(0)$.

We would like to have that if $\psi(x)$ and $V(x)$ are smooth, then

$$H\psi(x) = -\frac{1}{2} \Delta \psi(x) + V(x) \psi(x)$$

$=$ r.h.s. of (SE) in the usual sense.

<u>the aim of this course:</u>

- Remove the quotation marks from the above (up to references to text-books in functional analysis)
- Define "atomic" Hamiltonians
- Dynamics of multi-particle systems
- Wigner functions, and "geometrical optics" approximations in phase space
- Creation and annihilation operator formalism for bosons and fermions

1.2. Physical interpretation of QM

- Problem: Although distributed with probability density $|\psi(x,t)|^2$, the electrons arrive at the detector as well-localized "blobs", i.e., particles. What happens after they have passed the detector?

Conventionally solved by the

Projection postulate = "collapse of the wave function":

Suppose that the measurement device gives a "yes/no" answer to the question "Is the particle in region $B \subset \mathbb{R}^3$ at time $t=t_0$"

- If "yes", then future evolution ($t>t_0$) is obtained by solving (SE) with initial data
$$\psi_1(x,t_0) := \frac{1}{\left(\int_B dx\, |\psi_-(x,t_0)|^2\right)^{1/2}} \mathbb{1}(x\in B)\, \psi_-(x,t_0)$$
where $\psi_-(x,t)$ is the solution to (SE) for $0\le t\le t_0$.
[$\mathbb{1}(P) := 1$, if condition P is true, and $:= 0$ if false.]
- If "no", then use initial data
$$\psi_0(x,t_0) := \frac{1}{\left(\int_{\mathbb{R}^3\setminus B} dx\, |\psi_-(x,t_0)|^2\right)^{1/2}} \mathbb{1}(x\notin B)\, \psi_-(x,t_0)$$

- This is often enough in practical laboratory experiments, but an unsatisfactory answer in many other respects:

  * What counts as a measurement?
  * Leads to discontinuous & nonlinear time-evolution.
  * How to desribe the "particle + device"-system? (does somebody measure the measurement device?)

There have been many proposals for more complete explanations or descriptions for the collapse of wave function. If curious, look up the Wikipedia entry for "Interpretations of quantum mechanics".

Let us present here only two of them: GRW (Ghirardi, Rimini, Weber) theory and Bohmian mechanics. These two have the benefit of being mathematically complete descriptions. Below is a very brief summary; More details and discussion can be found from the lecture notes of a course by Tumulka, held at the Rutgers University (New Jersey, USA) in 2011. (Direct link available on the webpage of this course.)

1.2.1. GRW Theory

Idea: Measurements do not need a "measurer". Instead they happen spontaneusly, in a random manner.

In GRW theory, the collapse happens at times $(0<) t_1 < t_2 < \dots$ which are given by a Poisson process with rate λ. ($\Rightarrow$ the average time from one collapse to the next is an independent random variable with a mean $\frac{1}{\lambda}$.)
After each collapse, the particle will be found in a region whose size is determined by a new parameter σ and whose center is chosen randomly, according to the probability density $|\psi(x, t_i)|^2$.

$\Rightarrow \psi(x,t)$ is a well-def. stochastic process.

- The experimentally allowed values for the new parameters λ, σ are quite limited. Two possibilities would be

$$(\text{GRW}) \qquad \lambda \approx \frac{1}{10^{16}\,s}, \quad \sigma \approx 10^{-7}\,m$$

$$(\text{Adler}) \qquad \lambda \approx \frac{3}{10^{8}\,s}, \quad \sigma \approx 10^{-6}\,m$$

- $\Rightarrow$ collapses infrequent. But each particle has its own "clock" $\Rightarrow$ very frequent in macroscopic matter.

- Time-evolution not identical to (SE), even for free isolated particle. $\Rightarrow$ satisfies the standard projection only in approximation. $\Rightarrow$ experimentally testable consequences

1.2.2. Bohmian mechanics

(= De Broglie-Bohm theory (wikipedia)
= pilot-wave theory)

Idea: Add new dynamical variable $Q(t)$ which determine the position(s) of the particle(s) at t.

* Needs to be done consistently with the probability interpretation $\Rightarrow$ $Q(t)$ is random and distributed with density $|\psi(x,t)|^2$.

It suffices to assume that $Q(0)$ is a random variable with a distribution $|\psi(x,0)|^2 d^3x$. For any other times, its values can be found by solving the equation

$$\frac{d}{dt} Q(t) = \frac{\hbar}{m} \operatorname{Im} \left.\frac{\nabla \psi}{\psi}\right|_{(Q(t),t)} .$$

* Here ψ satisfies a standard (SE)
 $\Rightarrow$ can be solved independently of $Q(t)$

* Particles have trajectories. (although these are random ...)

* "Measurement" is understood in the usual classical manner, as conditioning the initial data $Q(0)$.

* No separation to "system" and "apparatus".

* Needs some adjustment to account for particle creation and annihilation in quantum field theories. See the QFT entry on the Bohmian mechanics Wikipedia -page for references.

1.2. Mathematics Toolbox

Assumed prerequisites:

* Analysis in $\mathbb{R}^d$, $d \geq 1$.

* Topology in metric spaces:
  open sets, closed sets and closure,
  dense sets, compact sets, neighbourhood

  Continuity: Let X, X' be metric spaces with metrics d, d'.
  $f: X \to X'$ is continuous if and only if $\forall \varepsilon > 0, x \in X\ \exists \delta > 0$ s.t. (such that)
  $$d(x,y) < \delta \Rightarrow d'(f(x), f(y)) < \varepsilon.$$

  Completeness: Every Cauchy sequence converges.

* Linear algebra:
  vector space, linear mappings, subspaces. In $\mathbb{R}^d$: matrices.

* Basic measure theory:
  Positive measures, Lebesgue measure on $\mathbb{R}^d$, (L^p-spaces)

  Recap of basic results, for proofs see for instance: Rudin, Real and complex analysis.

  a) Dominated convergence theorem:
  Let μ be positive measure on X
  Suppose $(f_n)_{n \in \mathbb{N}}$ is a sequence of measurable functions, $f_n: X \to \mathbb{C}$, s.t. for almost every (a.e.) $x \in X$
  $$f_n(x) \xrightarrow{n \to \infty} f(x) \quad \text{exists.}$$
  If $\exists g: X \to [0, \infty]$, measurable

s.t. $\int_{\mathbb{X}} \mu(dx)\, g(x) < \infty$ and

$|f_n(x)| \leq g(x) \quad \forall n \in \mathbb{N},\ x \in \mathbb{X}$

then the limit function f is measurable, $\int \mu(dx)\, |f(x)| < \infty$ and

$$\lim_{n \to \infty} \int_{\mathbb{X}} d\mu\, f_n = \int_{\mathbb{X}} d\mu\, f .$$

b) Hölder's inequality: Let $1 < p < \infty$, and define $q = \left(1 - \frac{1}{p}\right)^{-1}$. Let μ be a positive measure on $\mathbb{X}$.

Then for all $f, g : \mathbb{X} \to [0, \infty]$ measurable

$$\int_{\mathbb{X}} \mu(dx)\, f(x)\, g(x) \leq \|f\|_p \, \|g\|_q$$

where $\|f\|_p := \left[\int_{\mathbb{X}} \mu(dx)\, |f(x)|^p \right]^{1/p} \ (\in [0, \infty])$.

Note: usually applied to $F, G : \mathbb{X} \to \mathbb{C}$ with $f = |F|$, $g = |G|$ to estimate $\left| \int_{\mathbb{X}} \mu(dx)\, F(x)\, G(x) \right| \leq \int_{\mathbb{X}} d\mu\, fg$.

c) Suppose $1 \leq p \leq \infty$ and μ is a positive measure on $\mathbb{X}$. Then $\|f\|_p$ defines a norm on $L^p(\mu)$ which makes it into a complete normed space. In addition,

a) If $f_n \to f$ in norm, then $\exists$ subseq. $(n_k)_{k \in \mathbb{N}} \subset \mathbb{N}$ s.t. $\lim_{k \to \infty} f_{n_k}(x) = f(x)$ for a.e. $x \in \mathbb{X}$.

d) If $1 \leq p < \infty$, $\mathbb{X} = \mathbb{R}^d$, $\mu =$ Lebesgue, then $C_c(\mathbb{R}^d) = \{ f : \mathbb{X} \to \mathbb{C} \mid f \text{ continuous and } \operatorname{supp} f \text{ compact} \}$ is dense in $L^p(\mu) \equiv L^p(\mathbb{R}^d)$.

e) Fubini's Theorem:

Let μ, ν be positive measures on X, Y, respectively. Assume that X, Y are σ-finite: $\exists (X_n)_{n\in\mathbb{N}}, (Y_n)_{n\in\mathbb{N}}$ s.t. $\mu(X_n), \mu(Y_n) < \infty$ $\forall n$ and $X = \bigcup_n X_n$, $Y = \bigcup_n Y_n$.

- If $F: X \times Y \to \mathbb{C}$ is measurable (with respect to $\mu \times \nu$) and

$$\int_X \mu(dx)\left[\int_Y \nu(dy)\, |F(x,y)|\right] < \infty \qquad (*)$$

then

$$\int_X \mu(dx)\left[\int_Y \nu(dy)\, F(x,y)\right]$$
$$= \int_Y \nu(dy)\left[\int_X \mu(dx)\, F(x,y)\right]. \qquad (**)$$

- If $F: X \times Y \to [0,\infty]$ is measurable, $(**)$ holds also if $(*)$ is not true, in the sense that both iterated integrals are infinite.

Remarks: - Lebesgue measures μ_d on $\mathbb{R}^d$ are σ-finite, and $\mu_{d_1+d_2} = \mu_{d_1} \times \mu_{d_2}$ (more precisely, need to add some sets of measure 0.)
- Any function $F: \mathbb{R}^d \to \mathbb{C}$, which is a.e. a pointwise limit of a sequence of continuous functions, is Lebesgue measurable.

* If any of the above concepts or results sounds unfamiliar, look them up in Wikipedia or in a textbook (Rudin).

2. Hilbert spaces

2.1. Definition

$\mathcal{H}$ is called a Hilbert space if it satisfies all of the following:

* $\mathcal{H}$ is a complex vector space.

* $\mathcal{H}$ has a scalar product:

$$(\cdot,\cdot) : \mathcal{H} \times \mathcal{H} \to \mathbb{C} \quad \text{s.t.}$$

a) $(\phi, \psi)^* = (\psi, \phi)$
b) $(\phi, \psi_1 + \psi_2) = (\phi, \psi_1) + (\phi, \psi_2)$
c) $(\phi, \alpha\psi) = \alpha(\phi, \psi)$
$\forall \phi, \psi \in \mathcal{H}, \ \alpha \in \mathbb{C}$
d) $(\psi, \psi) \geq 0 \quad \forall \psi \in \mathcal{H}$.
e) $(\psi, \psi) = 0 \Rightarrow \psi = 0$.

* $\mathcal{H}$ is complete in the norm-topology given by

$$\text{(N)} \qquad \|\psi\| := \sqrt{(\psi, \psi)} \qquad \forall \psi \in \mathcal{H}.$$

Notes: • a) + b) + c) imply that $(\cdot,\cdot)$ is sesquilinear: it is linear in the second argument and conjugate-linear in the first argument.

2.2. Diversion: Norm and norm-topology.

Let V be a vector space. $\|\cdot\| : V \to \mathbb{R}$ is called a norm if

a) $\|\psi\| \geq 0 \quad \forall \psi \in V$
b) $\|\psi\| = 0 \Rightarrow \psi = 0$.
c) $\|\alpha\psi\| = |\alpha| \, \|\psi\| \quad \forall \alpha \in \mathbb{K}, \psi \in V$
d) $\|\psi + \phi\| \leq \|\psi\| + \|\phi\| \quad \forall \psi, \phi \in V$.

<u>Norm-topology</u> is the topology defined using the metric

$$d(\psi, \phi) := \|\psi - \phi\|.$$

<u>Continuity</u>: Let $\mathbb{X}$, $\mathbb{Y}$ be normed spaces. Then $F: \mathbb{X} \to \mathbb{Y}$ is continuous iff

$$\forall \psi \in \mathbb{X}, \varepsilon > 0 \quad \exists \delta > 0 \text{ s.t. } \|\phi - \psi\| < \delta \Rightarrow \|F(\phi) - F(\psi)\| < \varepsilon.$$

* If V is complete in the norm-metric, it is called a Banach space.

* <u>theorem</u> a) – e) $\Rightarrow$ $\|\cdot\|$ is a norm on $\mathcal{H}$.

Pf. d) $\Rightarrow$ $\|\psi\| \geq 0$ & e) $\Rightarrow$ $\|\psi\| = 0$ only if $\psi = 0$,
$\|\alpha\psi\|^2 = (\alpha\psi, \alpha\psi) = \alpha^*\alpha(\psi, \psi) = |\alpha|^2\|\psi\|^2$.
The triangle inequality is proven in th. 2.3. $\square$

* The set of <u>bounded</u> linear transformations of a normed space V is defined as

$$\mathcal{B}(V) := \{\Lambda: V \to V \mid \Lambda \text{ linear and } \|\Lambda\| < \infty\}$$

where $\|\Lambda\| := \sup\{\|\Lambda\psi\| \mid \psi \in V, \|\psi\| = 1\}$.

- $\Lambda: V \to V$ linear is called bounded whenever $\|\Lambda\| < \infty$.
- $\mathcal{B}(V)$ is also a normed space with the above norm $\|\cdot\|$.

<u>2.3. Theorem</u> Assume a) – e). Then

$\forall \psi, \phi \in \mathcal{H}$:

(i) $|(\phi, \psi)| \leq \|\phi\|\,\|\psi\|$ (Cauchy-Schwarz)

(ii) $\|\phi + \psi\| \leq \|\phi\| + \|\psi\|$

(iii) $\|\psi\| \leq \|\psi + \lambda\phi\| \quad \forall \lambda \in \mathbb{C}$ $\iff$ $(\phi, \psi) = 0$.

Proof: Let $\alpha = (\psi, \phi) \in \mathbb{C}$. Then $\forall \lambda \in \mathbb{C}$

$$(*) \quad \begin{cases} 0 \le \|\psi + \lambda\phi\|^2 = (\psi + \lambda\phi, \psi + \lambda\phi) \\ \quad = (\psi,\psi) + (\lambda\phi, \psi) + (\psi, \lambda\phi) + (\lambda\phi, \lambda\phi) \\ \quad = \|\psi\|^2 + |\lambda|^2 \|\phi\|^2 + (\psi, \lambda\phi) + (\psi, \lambda\phi)^* \\ \quad = \|\psi\|^2 + |\lambda|^2 \|\phi\|^2 + 2\,\mathrm{Re}(\lambda\alpha) \end{cases}$$

If $\phi = 0 \Rightarrow (\psi, \phi) = 0 \quad \forall \psi \in \mathcal{H} \quad$ ((c))
$\Rightarrow \|\phi\|^2 = (\phi, \phi) = 0 \Rightarrow$ (i) holds.
If $\phi \neq 0$, choose $\lambda = -\dfrac{\alpha^*}{\|\phi\|^2}$

$$\Rightarrow 0 \le \|\psi\|^2 + \frac{|\alpha|^2}{\|\phi\|^4}\|\phi\|^2 - 2\frac{|\alpha|^2}{\|\phi\|^2}$$

$$= \|\psi\|^2 - \frac{|\alpha|^2}{\|\phi\|^2} \Rightarrow |\alpha|^2 \le \|\psi\|^2 \|\phi\|^2$$

$\Rightarrow$ (i) holds.
Thus (i) has been proven. $\Rightarrow$

$$(\|\phi\| + \|\psi\|)^2 = \|\phi\|^2 + \|\psi\|^2 + 2\|\phi\|\,\|\psi\|$$
$$\underset{(i)}{\ge} \|\phi\|^2 + \|\psi\|^2 + 2|(\phi, \psi)|$$

But
$$\|\phi + \psi\|^2 = (\phi + \psi, \phi + \psi)$$
$$= \|\psi\|^2 + \|\phi\|^2 + 2\,\mathrm{Re}(\psi, \phi)$$
$$\le \|\psi\|^2 + \|\phi\|^2 + 2|\mathrm{Re}(\psi, \phi)|$$
$$\le \|\psi\|^2 + \|\phi\|^2 + 2|(\psi, \phi)|$$

Thus (ii) holds, as well.
To prove (iii), note that if $\alpha = 0 \Rightarrow$ (by $(*)$)

$$\forall \lambda \in \mathbb{C}: \|\psi + \lambda\phi\|^2 = \|\psi\|^2 + |\lambda|^2 \|\phi\|^2$$
$$\ge \|\psi\|^2 \Rightarrow \text{(iii) holds.}$$

If $\alpha \neq 0 \Rightarrow \phi \neq 0$ and thus by (i) and $(*)$

$$\|\psi + \lambda\phi\|^2 = \|\psi\|^2 - \frac{|\alpha|^2}{\|\phi\|^2} < \|\psi\|^2, \text{ for } \lambda = -\frac{\alpha^*}{\|\phi\|^2}.$$

$\Rightarrow$ (iii) does not hold. $\square$

2.4. Definitions: * From now on $\mathcal{H}$ denotes a Hilbert space.

* $\psi, \phi \in \mathcal{H}$ are <u>orthogonal</u>, denoted $\psi \perp \phi$, iff. $(\psi, \phi) = 0$.

* If $E \subset \mathcal{H}$ any set, its <u>orthogonal complement</u> is defined as
$$E^\perp = \{\psi \in \mathcal{H} \mid (\phi, \psi) = 0 \ \forall \phi \in E\}$$