

Introduction to Mathematical Physics Quantum Dynamics, fall 2013

Course information and announcements from department's webpages (wiki.helsinki.fi/display/mathstat/Opiskelu)

1. Motivation & introduction
Double-slit experiment

* Modern version in the attached paper. (movies of the result available in a supplement; Directs 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

(2)

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, must have

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

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

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

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

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

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

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

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

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 " \sim " in the following. Note that then

$$\Delta_{\tilde{x}} = 1 \leftrightarrow \Delta x = 10^{-10} \text{ m}, \quad \Delta_{\tilde{t}} = 1 \leftrightarrow \Delta t \approx 10^{-16} \text{ s}.$$

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

$$(SE) \quad i \partial_t \psi(x, t) = -\frac{\hbar^2}{2m} \Delta_x \psi(x, t) + V(x) \psi(x, t) .$$

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) must hold for all $t \geq 0$]

\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) $\Leftrightarrow \|\psi(t)\| = 1 \quad \forall t$
 $\Rightarrow \forall t \exists U(t): L^2 \rightarrow L^2$ 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
 $U(t+s) = U(t)U(s) \quad \forall t, s \geq 0$.
- Assume continuity of the time-evol.



in the following precise sense:

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

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

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

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

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.

The aim of this course:

- Remove the quotation marks from the above (up to references to textbooks in functional analysis)
- Define "atomic" Hamiltonians H .
- Discuss many-particle systems

optional topics (if time permits):

- Creation operator formalism of bosons and fermions
- Quantum statistical mechanics (random wave functions)

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 $0 \leq t \leq t_0$.
[$\mathbb{1}(P) := 1$, 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 describe 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 spontaneously, 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 $\ln(x, t_i) / \sigma^2$.

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

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

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

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

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

- o - 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 $|\psi(x,0)|^2 dx$. For any other times, its values can be found by solving the equation

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$$\frac{d}{dt} Q(t) = \frac{\hbar}{m} \operatorname{Im} \frac{\nabla \psi}{\psi} (Q(t), t)$$

* 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.