Week 0

PHY 303 Quantum Mechanics
Instructor: Sebastian Wüster, IISER Bhopal, 2021

These notes are provided for the students of the class above only. There is no guarantee for correctness, please contact me if you spot a mistake.

0 Administrative affairs

(i) Office: drop me an email to arrange a skype call
Office hours: tba.
Phone: 1213
Email: sebastian@iiserb.ac.in
webpage: http://home.iiserb.ac.in/∼sebastian/teaching.html

(ii) Literature:

- D. J. Griffiths, *Introduction to Quantum Mechanics* [GR] **the** textbook
- R. Shankar, *Principles of Quantum Mechanics*, [SH]
- J. J. Sakurai, *Modern Quantum Mechanics* [SA]

The course will mainly follow GR and SH. Where stray topics are taken from elsewhere I will try to indicate this.

(iii) Lectures and tutorials

- It is likely that the whole semester will remain in the online mode, however I shall attempt to offer the hybrid mode as soon as that is permitted. *(fully online mode)* Lectures will be provided as online video, based on screencapture explanation of these notes with mouse cursor, possibly with additional movies or presentation elements. Please download and view these early in the week, to be prepared to tackle assignments. *(hybrid mode)* Students willing and able to attend life classes can attend those, while a video+audio recording of the board and interaction is recorded and provided online for all others.
- I am arranging lecture notes into "week" segments, based on similar content. While most of those segments should indeed take a week for us to work through, this will not be true for all and they may take less or more often more time.
- There will be two weekly online sessions (i) One will be alternating between two different formats: (A) In one week we shall have a flipped classroom tutorial, conducted in the format of a parallel video chat session possibly paired with examineer life-quiz and a assignment-class where we discuss solutions to the assignments. In these we will do little tasks to understand the material more deeply. You will have to have gone through the lecture notes *prior* to the flipped classroom session. (B) The following week we shall do a TA-class/assignment class in which you explain the solutions of assignments to each

other. (ii) The second weekly (maybe bi-weekly) session will be a Q&A chat, where you can ask me or the TA questions on anything from the lecture, tutorials or assignments.

(iv) Assessment:

- **3 scheduled Quizzes: 13.33+13.33+13.33=40%** There will be some quizzes lasting 1-1.5 hours. These are "open notes" quizzes, so make your notes available offline or on a device beforehand. These will be proctored life and/or via camera. At the end, you have to camscan and upload your solution onto the teams page. Think of the second quiz as "mid-sem".
- **Assignments: 30%** There will be about five-seven assignments handed out with a two week deadline each. I expect you to form teams of 4-6 students and stick in these teams for the semester. Hand in only one solution per team. The TA is instructed to give full marks for *any serious attempt* at a given question of the assignment, even if the result is wrong. This is to discourage copying and encourage doing it yourself. However, the TA is asked to deduct marks for messy presentation and blatant copying from anywhere. The same teams will be used in tutorials, see below. Submit your final assignment solution via email to the TA. All has to be integrated in a single file, e.g. pdf. This may be a good opportunity to learn LaTex and nicely typeset your solution, but handwritten and good-quality scanned/photographed is fine too. *The mark will be from the best* $(N-1)$ *of* N *assignments.*
- **Numerics component of assignments:** Moderns science almost always necessitates the heavy use of computers. Most assignments will contain a numerics component, to be done using matlab. Please make the campus license version downloadable from the CC webpage available on at least one computer in your team. You shall also need VPN access to the campus network for the matlab license. For each assignment, I will provide a template code package that you have to only minorly edit. See notes on numerics assignments online. No prior experience of either programming or matlab should be required, but if you read some online notes regarding introduction to matlab in the first weeks, that might allow you to have more fun with this part of the assignments.
- **TA class and tutorial attendance: 10%** This will be compulsory, we record the sessions as thus see if you were present. When attendance is less than 60% the marks for this component are 0, and for more than 90% they are 100. In between they are as per fractional attendance.
- **Final exam: 20%** The exams will try to test understanding of the essential *physics* concepts taught, not maths. For guidance regarding what are the most important concepts look at the quizzes and assignments. All exams will be designed to give a significant advantage to those students that solved all assignments by *themselves* within their team. Exams will likely be conducted in the same way as quizzes.

0.1 Course Outline

PART 1 (PHY303)

1) **Motivation, foundations and review:** ∼ 3 weeks
   - Why do we need to know more about quantum mechanics than we learnt in PHY106? Review

of basic probability theory, linear algebra and function vector spaces. Schrödinger's equations, position versus momentum space. Expectation values.

2) **Solvable quantum problems in one dimension:** $\sim$ 3 weeks
• The square well potential, harmonic oscillator, tunneling, free particle

3) **Mathematical Interlude:** $\sim$ 2 weeks
• Commutators, simultaneous diagonalisation, generalised uncertainty principle, pictures for time-evolution

4) **Quantum mechanics in three dimensions:** $\sim$ 4 weeks
• Angular momentum, Hydrogenic atoms, spin, angular momentum additions

5) **Multi-particle systems:** $\sim$ 2 weeks
• indistinguishable particles, non-classical correlations

PART 2 (PHY304)

6) **Approximation methods for stationary states:**
• Time independent perturbation theory, variational method, WKB approximation

7) **Approximation methods for time-dependent phenomena:**
• Time dependent perturbation theory, Fermi's golden rule, adiabatic theorem

8) **Basic Gauge theory:**
• Charged particle in an electromagnetic field

9) **Quantum scattering theory:**
• Born approximation, partial wave decomposition

10) **Relativistic quantum mechanics:**

Contents

0.2 Math content

Moving from year 2 to year 3 at IISERB and into your physics major, you will experience a signifiant upwards jump of the level of mathematics in most courses, certainly in this one. I will expect you to be familiar with the following math topics:

- vectors, scalar-products, norm of vectors
- matrices, eigenvalues and eigenvectors of matrices
- Solutions of basic ordinary differential equations
- complex numbers
- basic differentiation and integration

Where you have doubts about being sufficiently familiar with any of those, please consult your math course notes, books or online resources. Focus on books/courses of the kind "mathematics for scientists and engineers" that tell you "how to actually get calculations done". An exemplary online resource is e.g. this link

For the following required math tools, I shall attempt to give a small self contained introduction:

- non-cartesian / curvilinear coordinate systems

- function vector spaces, advanced linear algebra
- solutions of partial differential equations
- boundary value problems, solutions through power series
- Dirac delta function

1 Motivation, foundations and review

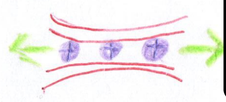
1.1 Motivation

- You have learnt in PHY106 that the concepts of classical physics are unable to explain the details of a couple of key experiments/phenomena, such as the photo-effect, black-body radiation and the stability of the atom. We will not repeat discussions of these historical developments and experiments here, please revisit PHY106 week 4,5 for all items you might have forgotten.
- To make room for that presentation of historical developments, and to reflect the fact that PHY106 is taken by all IISERB students (also non PHY/MTH majors), we had reduced the emphasis on the mathematical formalism there to a large extent.
- This course will introduce the math behind quantum mechanics in much greater depth, and then revisit all the key scenarios you already briefly encountered in PHY106 in detail. Essentially, whereever earlier we had just shown you results without proof, now we will show you the "why".
- Very important examples for which we will supply derivations missing earlier are Eq. 107(c) (PHY106, week 8), the quantum harmonic oscillator (PHY106, week 9) and the Hydrogen wave functions (PHY106, week 10) [1].
- Another major aspect that deserves much more attention, is the handling and interpretation of measurements in quantum mechanics.
- I also encourage you to re-watch the videos I had given you for PHY106, since quite a few aspects of those were not yet touched upon by that course, but some more will be now:
  Powers of ten
  The secrets of quantum physics
  Quantum theory made easy (part I)
  Quantum theory made easy (part II)
  Many explanations in these movies are too fast and others too basic. However they communicate that quantum mechanics is exciting and mind-boggling.

[1] I shall refer to the material of PHY106 frequently, please refer to my webpage (2019-20-II Semester)

Quantum information

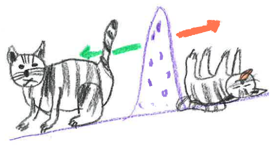
- Entanglement
- Quantum computation



- Quantum cryptography

Decoherence and quantum classical transition

- Schrödinger's cat
- Why the world around us appears classical



Spectroscopy and probing

- NMR, Tunneling microscope
- Lasers

Quantum statistical physics

- Bose-Einstein condensates
- degenerate Fermi gases

The bubble diagram here gives an idea of the central role played by "quantum mechanics" throughout most of modern physics.

PHY303 Quantum mechanics

- Bound states, discrete energies
- Quantum superpositions
- Wavepackets
- Angular momentum addition
- Entanglement
- Quantum mechanical measurement

Atomic, molecular and optical physics

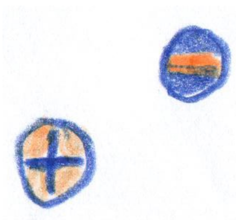
- Periodic table
- Molecular bonds
- Quantum optics

Solid state and material science

- quantum materials
- band structure, phonons,
- quasiparticles, excitons, magnons, plasmons
- magnetism, superconductivity

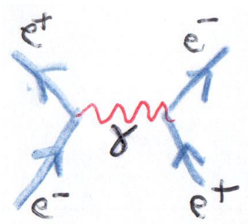
Relativistic quantum mechanics

- Dirac equation
- Spin
- Anti-particles



Quantum Field theory

- Gauge principle
- Particle creation and conversion



Nuclear and particle physics

- Super heavy elements, Nuclear fusion
- Neutron stars
- Exotic particles

1.2 Research frontier

- Pretty much all the advanced topics mentioned in the previous diagram are at the current research frontier with lots of activity.
- However even among the central box, i.e. the formalism of quantum mechanics and hence the present course, there are open questions, such as
  - How can we better describe a measurement in the quantum mechanical formalism?
  - How can we overcome the exponential scaling of a many-body Hilbertspace in computational approaches?
  - Is there some criterion that delineates macroscopic bodies behaving classically and microscopic ones quantum mechanically, or do really all bodies behave quantum mechanically? See e.g. this video .

1.3 Fundamental extensions of quantum mechanics (not in this course)

Already some flashed in previous boxes...

- In this lecture we will restrict ourselves to non-relativistic quantum mechanics, with velocities $v \ll c$, or energies $E \ll mc^2$. However quantum mechanics can be formulated adhering to the laws of special relativity and is then called "relativistic quantum mechanics", we will peep into this topic at the end of PHY304, or it would be more thoroughly covered in particle physics or quantum field theory lectures.
- We will also focus on single particle or few particle physics. Quantum mechanics usually requires advanced solution methods to deal with truly many particles, as for example required in condensed matter physics or quantum chemistry.
- Both concepts (relativity and many particles or uncertain particle numbers) are then combined in lectures on "quantum field theory".
- You recover classical mechanics from quantum mechanics in the limit $S/\hbar \to \infty$, as I shall mention occasionally. Also see week 11 of the PHY305 "classical mechanics" lecture notes on my webpage (only at the end of this semester, if you are interested).

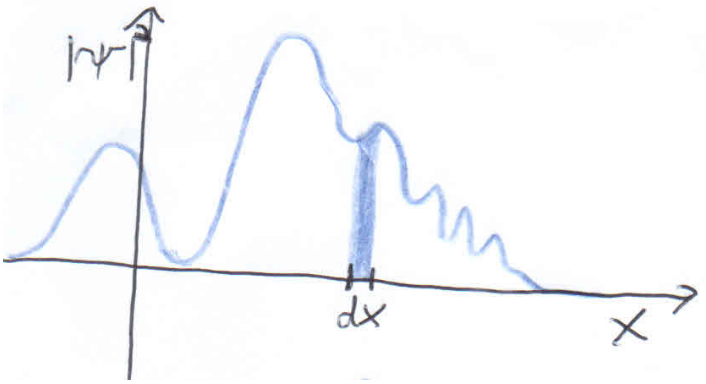
1.4 From classical to quantum mechanics

This section is a brief reminder or summary of PHY106, and intended as motivation for the math background in section 1.5.

The state of a particle: In classical mechanics we know everything about a particle if we specify its position $\mathbf{x}(t)$ and velocity $\mathbf{v}(t)$ (or momentum $\mathbf{p}(t)$). In PHY106 you learnt about a few key experiments (the photo effect, black body radiation, Compton scattering etc.) that forced us to develop quite different ideas. Instead of the above, all particles are in fact at the same time also waves. These are called matter waves. Mathematically we replace a well defined position and velocity by the

Wavefunction (or quantum state) of the particle. We shall write $\Psi(x,t)$ for a generic wavefunction that depends on one spatial coordinate x and time t.

- $\Psi(x,t)$ is a probability wave. That means that we consider $|\Psi(x,t)|^2 dx$ as the probability to find the particle in a small interval dx near the position x, see figure below. We say that $\rho(x,t) = |\Psi(x,t)|^2$ is the probability density for a measurement of the position of the particle (see section 1.5.2) at time t.



left: Exemplary probability density of particle position, for a particle with wavefunction $\Psi(x,t)$.

- Please review PHY106 weeks 5,6 for the reasons why we arrived at this picture. In short: To explain all experiments one has to attribute wave properties also to particles. The probability interpretation is then one that simply works, however there are a few aspects with which people have misgivings.
- Note that the wavefunction itself is a complex function, so by itself it cannot be related to a probability.

Dynamics of a particle: To find how the classical state $(\mathbf{x}(t), \mathbf{p}(t))$ changes in time, we can use Newton's equation

$$m\ddot{\mathbf{x}}(t) = \mathbf{F} = -\boldsymbol{\nabla} V(\mathbf{x}), \tag{1.1}$$

where m is the particle mass, $\mathbf{F}$ is the force, given by the gradient $\boldsymbol{\nabla}$ of the potential $V(\mathbf{x})$. The corresponding equation of motion for the wave function in quantum mechanics is

Schrödinger's equation (time dependent Schrödinger equation, TDSE), given by

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t). \tag{1.2}$$

- The TDSE is of first order in time derivatives. This means we can solve it as an initial value problem:

If we know the initial wavefunction $\Psi(x, t = 0)$, the equation uniquely determines the wavefunction $\Psi(x, t)$ at all later times.

- The left hand side contains the imaginary unit i, we thus require complex numbers to solve it. It also contains the reduced Planck's constant $\hbar = h/(2\pi) = 1.0546 \times \times 10^{-34}$ Js, where Planck's constant h is

$$h = 6.626 \times 10^{-34} \text{ Js.} \tag{1.3}$$

It has units of "Energy × times", which you shall learn in PHY305 is called an action. We shall see that for actions S of a problem with $S \sim \hbar$, quantum effects such as discrete energy states are usually crucial, while for $S \gg \hbar$ one recovers classical mechanics.

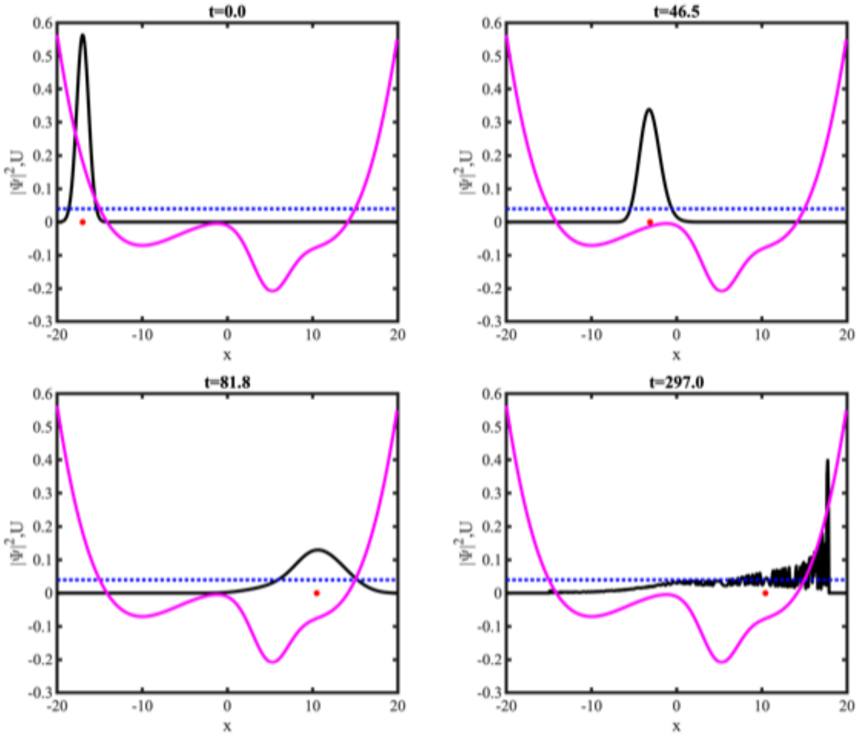
- In the same way that one cannot derive Newton's equation from any deeper principles, that is also not possible for Schrödinger's equation (1.2). However we went through some argumentation in PHY106 why the equation is reasonable to describe matter waves.

- We will see later, than one usually starts quantum mechanics by assuming its validity (and a few other so-called postulates). So far, the equation has passed every single experimental test.

- While the description of physics appears entirely distinct from Newtonian mechanics, the TDSE entails all the same essential physics (see example below), plus some new features, due to interference (which is only possible for waves).

Even in one dimension, analytical solutions of (1.2) can be found only for a few special cases, we will cover almost all of these in this lecture. However it is straightforward to solve it on a computer. Please revisit the following example in week 8 of PHY106

Example 1, Numerical solution of Schrödinger's equation: In the frames at different times below, we show $V(x)$ (magenta) $|\Psi(x,t)|^2$ (black), E (blue dashed) and $x(t)$ from Newton's equation (red dot).



This course will teach you how to solve this, but for now the message is only that the "location" of the particle actually follows the same rules. In addition to that, quantum mechanics can have a time varying uncertainty, and, in the last frame, interference effects. Please see the full movie on the webpage.

Interpretations of quantum mechanics:

According to the above, the wavefunction $\Psi(x,t)$ only gives us probabilistic information about the particle, in contrast to the certainties that we are used to from classical mechanics. This has been irritating scientists for long, and still does, leading to several different so-called "interpretations of quantum mechanics"[2] Suppose we had a particle in wavefunction $\Psi(x,t)$ and measured it to be at location x_0. We now want to ask "where was the particle before the measurement". Following Griffith, the main interpretations then differ as follows

(i) Realist: It already was at x_0, but we somehow could not know. In this interpretation, we assume quantum mechanics is just not all of the truth, and probabilities $\rho(x)$ arise due to incomplete information (or so called "hidden variables").

(ii) Orthodox (Copenhagen interpretation): The particle was nowhere specific. Only through the act of measurement do we force it to take a specific position. This position later remains

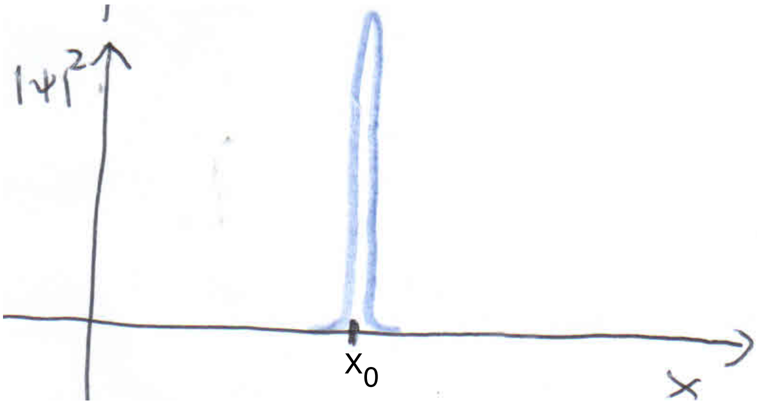
[2] As opposed to "math of quantum mechanics". Of that, there is only one, and it works.

re-producable (if we measure the position again) $^{(*)}$. This interpretation attributes a very special role to the act of measurement, why a "measurement" would be so special is still unresolved.

(iii) Agnostic: One does not want to worry about it, since it is logically impossible to measure what the position of the particle before the measurement was.

We shall follow (ii) here, as is usually done, since local realism (hidden variable theories) have been rules out by many experiments based on Bell's theorem, which we shall briefly visit in chapter 5.

In order to ensure $^{(*)}$ above, that measurements once done are reproducable afterwards, one has to assume the collapse of the wavefunction. If a particle had a wavefunction as in the figure on page 9, we then measure its position to be x_0, the measure changes the wavefunction to one very sharply peaked around x_0 as shown below.



left: Suppose a particle had the wavefunction on page 9, and then we measured it to be at position x_0. The act of measurement has collapsed the wavefunction to the one shown, peaked around x_0 up to the measurement resolution.

Again, this behaviour cannot be derived but has to be postulated, and describes all available experiments. The fact that measurements perturb quantum states in general, is central to quantum mechanics.