Quantum Mechanics

Week 2

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Exercise Material

Webpage

Week 1

Welcome to QM!

Organisational

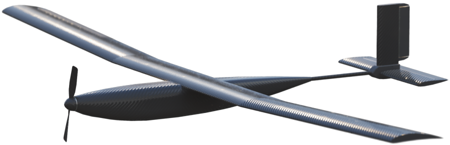
Review

Clicker Questions

Problem Set Hints

Welcome to QM!

- Sixth Semester Bachelor Student
- Member of Focus Project NOCTUA



Organisational

Structure

- **Lecture**: Wednesday 14:15-16:00 HG E7
- **Exercise**: Wednesday 16:15-18:00 HG D3.2
- **Textbook**: "Introduction to Quantum Mechanics" 3rd edition by David J. Griffiths.
- **For you every Week**:
  - Theory Sheet
  - Slides
  - Problem Set

Personal Recommendations

- Visit the exercise class
- Book is only worth it if you want to get a deeper understanding
- Problem Set difficulty is really similar to the one in the final exam
- Recognize that QM poses conceptual challenges. It's not always necessary to grasp every detail immediately; sometimes, accepting certain concepts initially can pave the way for understanding them more thoroughly later on.
- I would recommend using Tim Reinhart's Cheatsheet
- Utilize the Useful Information Sheet (UIS) provided on Moodle for the Problem Sets. This sheet will also be provided during the exam.

Midterm

- We will have a **non-mandatory** Midterm around April 24th (date to be confirmed).
- The Midterm will contribute 20% to the final grade only if it surpasses the grade obtained in the final exam.
- The Midterm will be a 60-minute assessment.

Exercise Structure

First Hour	Break	Second Hour
Lecture Review		1. Collaborative Problem-Solving
Clicker Questions		2. Solo Problem-Solving with Assistance
Problem Hints		3. Practice with Exam-Style Questions

Feel free to choose how you'd like to spend the second hour of the exercise session! And remember, I'm here to support your understanding, so don't hesitate to ask questions!

Review

Lecture 1

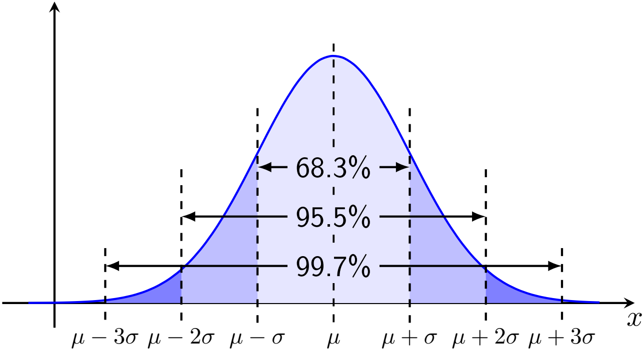
- Black-body radiation $\rightarrow$ Demonstrates quantization of energy.
- Double-slit diffraction of light $\rightarrow$ Exhibits wave behavior of light.
- Photoelectric effect $\rightarrow$ Demonstrates particle behavior of light.

Classical physics fails to fully explain certain phenomena, necessitating the development of a new framework for understanding.

Statistics

The important things we have to keep in mind are:

- **Average** $\equiv \langle x \rangle$
- **Squared Mean** $\equiv \langle x^2 \rangle$
- **Variance (Var)** $\equiv \langle x^2 \rangle - \langle x \rangle^2 = \sum (x - \langle x \rangle)^2 p(x)$
- **Standard Deviation** $\sigma \equiv \sqrt{\mathsf{Var}} = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$


68.3%
95.5%
99.7%
x
$\mu - 3\sigma$
$\mu - 2\sigma$
$\mu - \sigma$
μ
$\mu + \sigma$
$\mu + 2\sigma$
$\mu + 3\sigma$

The Schrödinger Equation (SE/TDSE)

$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t)}$$

Where

$\hbar \equiv \dfrac{h}{2\pi}$; $\quad m \equiv$ Mass of particle (mostly m_e); $\quad t \equiv$ time; $\quad x \equiv$ Position

$\Rightarrow$ Solving the TDSE gives you $\Psi(x,t) \equiv$ Wave function of the particle, **it has no physical meaning**

Wave Function

As seen in Analysis 3, a partial differential equation (PDE) can have multiple solutions. In our case, we focus on solutions within the subspace L^2, constituting a Hilbert Space.

Thus, for them to be **physically meaningful**,
they must be both $\underbrace{\textbf{square-integrable}}_{1}$ and $\underbrace{\textbf{normalized}}_{2}$.

- **1. Square Integrable**:

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2 \, dx < \infty}$$

- **2. Normalized**:

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2 \, dx = 1}$$

A direct consequence of these conditions is: $\Psi(x \to \pm\infty, t) = 0$.

These two conditions ensure that we only consider solutions that contain valid or physically meaningful answers.

The wave function is a complex function that can be expressed as $\Psi = u + iv$, where u and v are real-valued functions, and its complex conjugate is given by $\Psi^* = u - iv$

Remark: $\Psi^* \cdot \Psi = |\Psi|^2 = u^2 + v^2$

Statistical Interpretation

The **probability density** of the wave function is given by $|\Psi|^2 = \Psi^* \cdot \Psi$. To determine the probability of finding the particle between points a and b at time t_0, we integrate as follows:

$$\boxed{P(a < x < b) = \int_a^b |\Psi(x, t_0)|^2, dx}$$

Remark: It has been demonstrated in the lecture that if we normalize Ψ at time $t = 0$, it will remain normalized for all t

In probability theory, the expectation value, denoted $\langle A \rangle$, represents the average/mean outcome of a random variable or observable. It's calculated as:

$$\boxed{\langle A \rangle = \int \Psi^*(x) \hat{A} \Psi(x) \, dx}$$

$\langle A \rangle$ provides the average outcome in an ensemble.

An **ensemble** is a conceptual/mathematical model consisting of multiple virtual replicas of a system, all sharing the same initial conditions. Each replica represents a possible state that the real system could adopt.

Therefore $\Psi(x,t)$ has **no physically meaning** but $|\Psi(x,t)|^2$ **does**.

Observables and Operators

- **Observable** A: Is a characteristic of a physical system that we can measure. It represents what we're interested in learning about the system, such as its position or momentum.

- **Operator** $\hat{A}$: Is a mathematical function that represents the action of measuring an observable. It operates on the wave function of the system, extracting information about the observable being measured.

To determine the expectation value of an observable, we utilize the operator within the **"sandwich integral"** framework, as discussed before:

$$\boxed{\langle A \rangle = \int \Psi^*(x) \hat{A} \Psi(x), dx}$$

The operator acts on the wave function on the right-hand side.

In Quantum Mechanics, any observable and its corresponding operator can be expressed as a function of the position operator $\hat{x}$ and the momentum operator $\hat{p}$. Therefore, we can write $\hat{Q}$ as $\hat{Q} = \hat{Q}(\hat{x}, \hat{p})$ and their Observables $Q = Q(x, p)$.

Observable	**Operator**	**Expectation Value**
x	$\hat{x}$	$\langle x \rangle = \int \Psi^* x \Psi$
$p = mv$	$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	$\langle p \rangle = \int \Psi^* (-i\hbar\frac{\partial}{\partial x})\Psi$
E_{kin}	$\hat{E}_{kin} = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$	$\langle E_{kin} \rangle = \int \Psi^* (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2})\Psi$

Every observable quantity in classical mechanics is represented in QM by a linear Hermitian operator

Ehrenfest Theorem

The Ehrenfest Theorem states that the expectation values follow classical mechanics, thus:

$$\boxed{\langle v\rangle = \frac{d\langle x\rangle}{dt} \quad \rightarrow \quad \langle p\rangle = m\frac{d\langle x\rangle}{dt}}$$

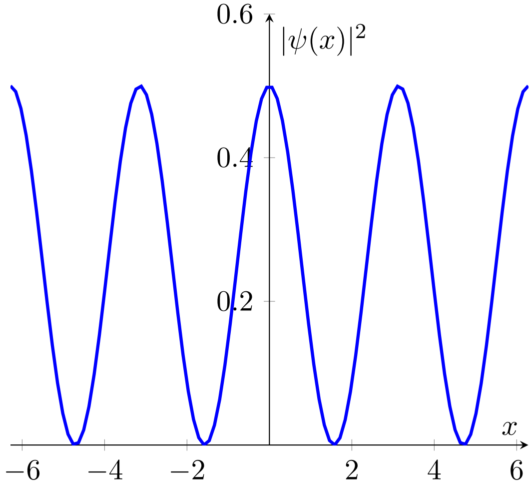
Uncertainty Principle

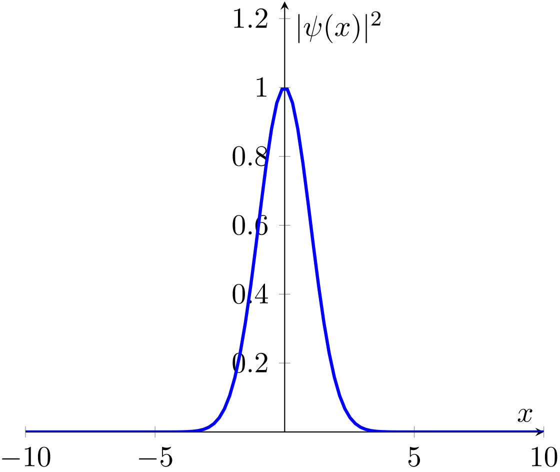
The Heisenberg Uncertainty Principle asserts that we cannot precisely determine both the position and momentum of a particle **simultaneously**.

Mathematically, this principle dictates that the product of their standard deviations must exceed $\frac{\hbar}{2}$, as shown below:

$$\boxed{\sigma_x \cdot \sigma_p \geq \frac{\hbar}{2}}$$

Remark: The following plots shown are an extreme case to help understand the Heisenberg principle; they are not valid solutions.


0.6
0.4
0.2
$|\psi(x)|^2$
x
-6
-4
-2
2
4
6


1.2
1
0.8
0.6
0.4
0.2
$|\psi(x)|^2$
x
-10
-5
5
10

Clicker Questions

Problem Set Hints

This week, our primary focus will be on exercises 1, 2, and 4.

Exercise 1

Consider the Gaussian distribution, $\rho(x) = Ae^{-\lambda(x-a)^2}$, where A, a, and λ are positive real constants.

1. If ρ is a normalized probability density, determine A.
2. Find $\langle x \rangle$, $\langle x^2 \rangle$, and σ_x.
3. Sketch the graph of $\rho(x)$.

Hint: $\int_{-\infty}^{\infty} f_{odd} dx = 0, \qquad \int_{-\infty}^{\infty} f_{even} dx = 2\int_{0}^{\infty} f_{even} dx$

Exercise 2

Consider the wave function, $\Psi(x,t) = Ae^{-\lambda|x|}e^{-i\omega t}$, where A, λ, and ω are positive real constants.

1. Normalize $\Psi(x,t)$.
2. Determine the expectation values of x and x^2.
3. Find σ_x, sketch the graph of $|\Psi(x,t)|^2$ as a function of x, and mark the points $(x = +\sigma_x)$ and $(x = -\sigma_x)$. What is the probability that the particle would be found outside this range?

Hint: $\Psi^* =$ Conjugate of Ψ, $\quad p(x) = \Psi^*(x,t) \cdot \Psi(x,t) = |\Psi(x,t)|^2$

Exercise 4

Hint: $\lambda = \frac{h}{p}, p = \sqrt{3mk_BT} \Rightarrow \lambda = \frac{h}{\sqrt{3mk_BT}} > d \Rightarrow T < \frac{h^2}{3mk_Bd^2}$

Questions?

THANK YOU!