PHYS 3386: QUANTUM MECHANICS 2

(WINTER 2024)

Professor (this week)

Best way to reach me!

Dr. Andreas Shalchi
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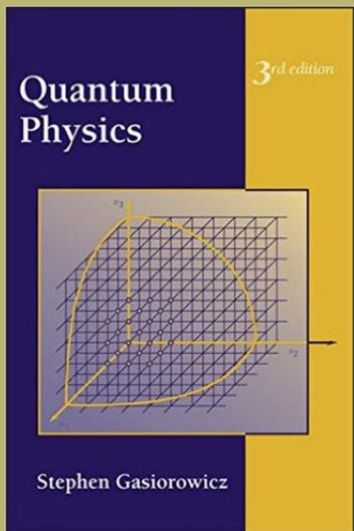
Classes:
Mondays, Wednesdays & Fridays 9:30-10:20,
527 Buller

Office Hours:
Mondays and Fridays 13:30-14:30

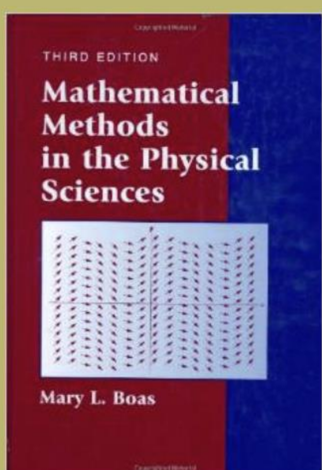
Course Website:
www2.physics.umanitoba.ca/u/shalchi/PHYS3386

Course Website

Textbook:



Mathematics:



PHYS 3386
Quantum Mechanics 2
Winter Term 2021

NEWS AND ANNOUNCEMENTS:

First class is on January 18th via ZOOM!

Links:

Lecture Notes

Homework Assignments

Application for Physics Computer Account

Math Tables

Declaration Form

Schedule A Document

Professor:

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219 Allen Bldg
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Lectures:
Monday, 9:30-10:20
Wednesday, 9:30-10:20
Friday, 9:30-10:20

Consultation times:
NA

Tutorials:
NA

Course Notes

Will be posted online the night before the lecture on the website!

PHYS 3386: Quantum Mechanics 2 - Lecture Notes (pdf files)

Introduction (January 18th)

Introduction (Recorded)

Lecture notes

Policies/Evaluation

Information About Voluntary Withdrawal:
Note that Voluntary Withdrawal has a number of impacts. The student must request permission to retake the course and there are limits to the number of repeated attempts. Access for VW students to the course may be limited if the course is full. A Voluntary Withdrawal shall be recorded on the Student History and Official Transcript issued by the University.

Final grades for courses in which Students ceased attending, without an official VW, will be included on the Student History and Official Transcript issued by the University, and will be factored into the Student's Grade Point Average.

Plagiarism and Cheating (University of Manitoba Undergraduate Calendar, p. 27):
To plagiarize is to take ideas or words of another person and pass them off as one's own. In short, it is stealing something intangible rather than an object. Obviously it is not necessary to state the source of well-known or easily verifiable facts, but students are expected to acknowledge the sources of ideas and expressions they use in their written work, whether quoted directly or paraphrased. This applies to diagrams, statistical tables and the like, as well as to written material, and materials or information from Internet sources. To provide adequate documentation is not only an indication of academic honesty but also a courtesy which enables the reader to consult these sources with ease. Failure to do so constitutes plagiarism. It will also be considered plagiarism and/or cheating if a student submits a term paper written in whole or in part by someone other than him/herself, or copies the answer or answers of another student in any test, examination, or takehome assignment.

Plagiarism or any other form of cheating in examinations or term tests (e.g., crib notes) is subject to serious academic penalty (e.g. suspension or expulsion from the faculty or university). A student found guilty of contributing to cheating in examinations or term assignments is also subject to serious academic penalty.

Policies/Evaluation

Examinations: Personations (University of Manitoba Undergraduate Calendar, p. 26):
A student who arranges for another individual to undertake or write any nature of examination for and on his/her behalf, as well as the individual who undertakes or writes the examination, will be subject to discipline under the university's Student Discipline Bylaw, which could lead to suspension or expulsion from the university. In addition, the Canadian Criminal Code treats the personation of a candidate at a competitive or qualifying examination held at a university as an offence punishable by summary conviction. Section 362 of the Code provides:

Personation at Examination
362. Everyone who falsely, with intent to gain advantage for him/herself or some other person, personates a candidate at a competitive or qualifying examination held under the authority of law or in connection with a university, college or school or who knowingly avails him/herself of the results of such personation is guilty of an offence punishable on summary conviction. 1953 54,c.51,s.347.

Both the personator and the individual who avails him/herself of the personation could be found guilty. Summary conviction could result in a fine being levied or up to two years of imprisonment.

Faculty of Science Statement on Academic Dishonesty:
The Faculty of Science and The University of Manitoba regard acts of academic dishonesty in quizzes, tests, examinations, laboratory reports or assignments as serious offences and may assess a variety of penalties depending on the nature of the offence.

Acts of academic dishonesty include, but are not limited to bringing unauthorized materials into a test or exam, copying from another individual, using answers provided by tutors, plagiarism, and examination personation.

Note: cell phones, pagers, PDAs, MP3 units or electronic translators are explicitly listed as unauthorized materials, and must not be present during tests or examinations.

Policies/Evaluation

Note: cell phones, pagers, PDAs, MP3 units or electronic translators are explicitly listed as un-authorized materials, and must not be present during tests or examinations.

Penalties that may apply, as provided for under the University of Manitoba's Student Discipline ByLaw, range from a grade of zero for the assignment or examination, failure in the course, to expulsion from the University. The Student Discipline ByLaw may be accessed at:

http://umanitoba.ca/admin/governance/governing_documents/students/868.htm

Suggested minimum penalties assessed by the Faculty of Science for acts of academic dishonesty are available on the Faculty of Science webpage:

http://umanitoba.ca/faculties/science/resources/Discipline__Penalties_Table_Jul09.pdf

All Faculty members (and their teaching assistants) have been instructed to be vigilant and report all incidents of academic dishonesty to the Head of the Department.

Schedule A:

A Schedule A document is posted on http://www2.physics.umanitoba.ca/u/shalchi/PHYS3386/. This is a Policy and Resource Document with information on various University and Unit policies regarding academic integrity, student discipline, and respectful learning environment, for example, and on academic and student supports that are available, including a statement regarding mental health with referral information to the Student Counselling Centre and University Health Services.

Student Accessibility Services (SAS)

If you are a student with a disability, please contact SAS for academic accommodation supports and services such as note-taking, interpreting, assistive technology and exam accommodations. Students who have, or think they may have, a disability (e.g. mental illness, learning, medical, hearing, injury-related, visual) are invited to contact SAS to arrange a confidential consultation.

Student Accessibility Services
520 University Centre
204 474 7423
http://umanitoba.ca/student/saa/accessibility/
Student_accessibility@umanitoba.ca

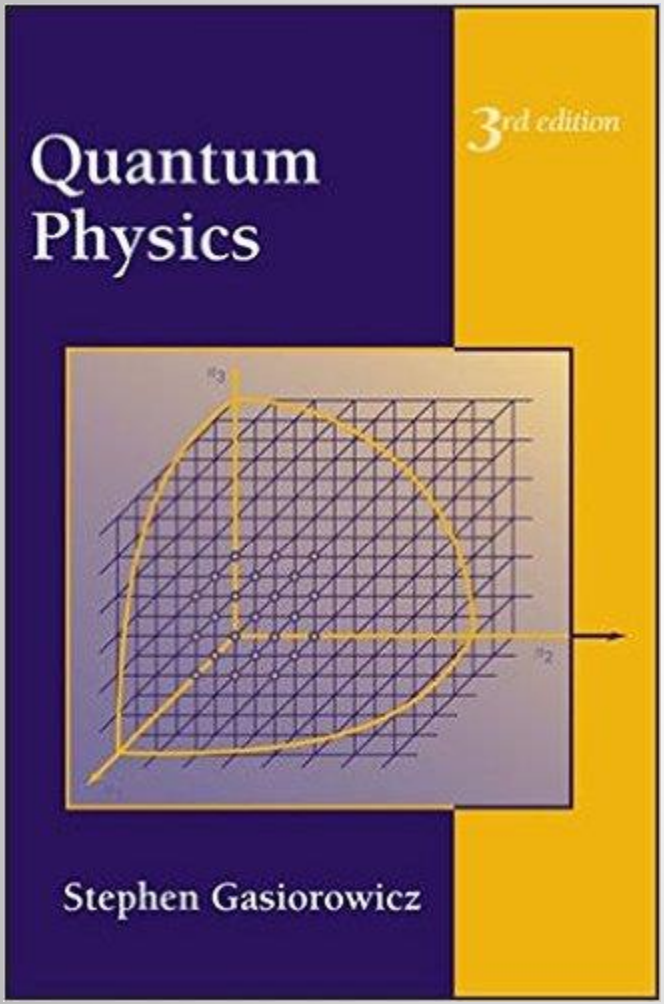
IN THE CASE OF A FIRE ALARM:

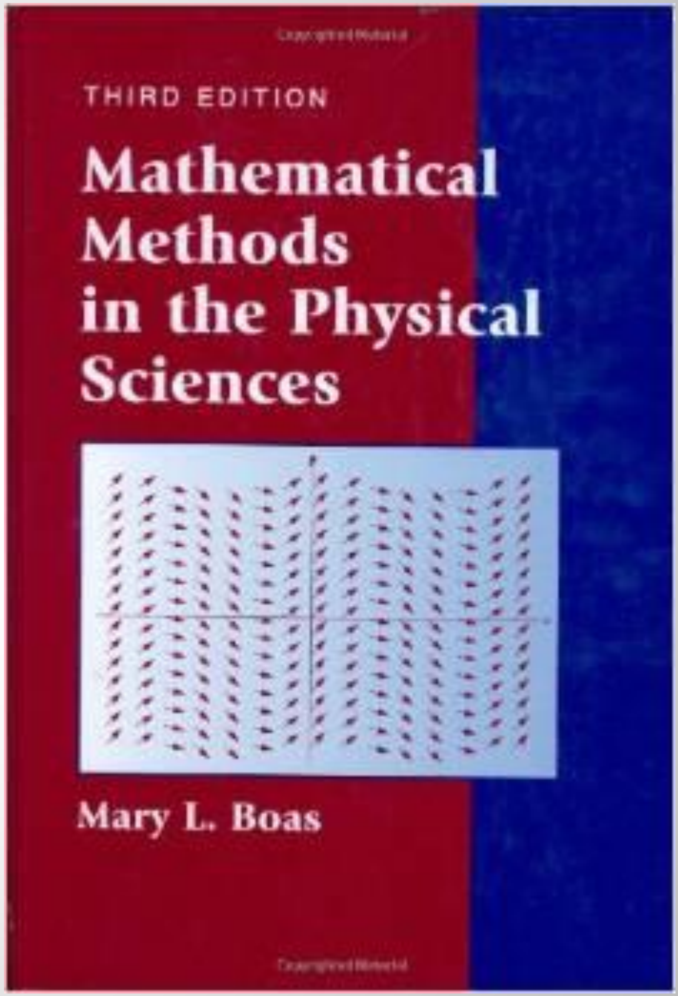
- **Remain calm**
  - if it is safe, evacuate the classroom or lab
  - go to the closest fire exit
  - do not use the elevators
- **If you need assistance to evacuate the building, inform your professor or instructor immediately.**
- **If you need to report an incident or a person left behind during a building evacuation, report it to a fire warden or call security services 204-474-9341.**
  - **Do not** reenter the building until the **"all clear"** is declared by a fire warden, security services o the fire department.
- **Important: only those trained in the use of a fire extinguisher should attempt to operate one!**

faculty of SCIENCE
discover the unknown + invent the future

University of Manitoba

Textbooks


3rd edition
Quantum
Physics
Stephen Gasiorowicz


THIRD EDITION
Mathematical
Methods
in the Physical
Sciences
Mary L. Boas

Course Outline

(A detailed course schedule will be part of the ROASS!)

1) Introduction and Review of Quantum Mechanics I *
2) The General Structure of Wave Mechanics (Book Chapter 5)
3) Operator Methods in Quantum Mechanics (Book Chapter 6)
4) Angular Momentum (Book Chapter 7)
5) Three Dimensions and the Hydrogen Atom (Book Chapter 8)
6) Matrix Representation of Operators (Book Chapter 9)
7) Spin (Book Chapter 10)
8) Time-Independent Perturbation Theory (Book Chapter 11)
9) The Real Hydrogen Atom (Book Chapter 12)
10) Introduction to Relativistic Quantum Mechanics

*** This refers to the course PHYS 2386: *Introduction to Special Relativity and Quantum Physics***

Review of Quantum Mechanics I

- Different Descriptions of Quantum Mechanics (QM)
  - Wave Mechanics:

    Electrons and other particles are described by wave equations such as Schrödinger's equation (1926). The mathematical formulation is very similar compared to other waves (e.g., sound waves, electromagnetic waves).

  - Matrix Mechanics:

    Describes QM based on operators and matrices. It was developed by Heisenberg, Born, and Jordan in 1925. Pauli derived the hydrogen atom spectrum in 1926 before the development of wave mechanics.

  - Path Integrals (is more advanced, not discussed in 3386):

    Describes QM based on functional integrals also known as Wiener integrals. This formulation was introduced into QM by Feynman and Dirac. Each path is possible but with a different probability.

Review of Quantum Mechanics I

- Wave Mechanics and Wave Equations
  - Schrödinger's Equation: non-relativistic particles without spin

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi + V\Psi$$

Laplace operator

  - Pauli's Equation: non-relativistic particles with spin
  - Klein-Gordon Equation: relativistic particles without spin

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\Psi - \Delta\Psi + \frac{m^2c^2}{\hbar^2}\Psi = 0$$

  - Dirac's Equation: relativistic particles with spin

$$i\hbar\frac{\partial}{\partial t}\Psi = c\sum_{n=1}^{3}\alpha_n\hat{p}_n\Psi + \beta mc^2\Psi$$

Review of Quantum Mechanics I

- Principles of Wave Mechanics

  - Assume that particles are described by a wave Ψ rather than a classical trajectory

$$\vec{r}(t) \quad \rightarrow \quad \Psi\left(\vec{r}, t\right).$$

  - The probability density to find the particle at a certain time and position in space is then $\Psi\Psi^*$. ← complex conjugate

  - Note the similarity with statistical physics!

  - Linear waves have the form

$$\Psi\left(\vec{r}, t\right) \propto e^{i(\vec{k}\cdot\vec{r}-\omega t)}.$$

Review of Quantum Mechanics I

- <u>Derivation of Schrödinger's Equation</u>
  - The energy of a non-relativistic particle is given by

$$E = \frac{p^2}{2m} + V(\vec{r}, t).$$

  - Use the <u>de Broglie relations</u> (1924)

$$E = \hbar\omega \qquad \text{and} \qquad \vec{p} = \hbar\vec{k}.$$

  - This gives us the relation between frequency ω and wave number k

$$\hbar\omega = \frac{\hbar^2}{2m}\vec{k}^2 + V(\vec{r}, t).$$

  - Assume there is an equation for the wave function Ψ. This equation must contain only <u>first derivatives wrt time</u>. Only then the theory is deterministic. Note, deterministic means that if we know the initial wave function, we are able to compute the wave for any later time.

Review of Quantum Mechanics I

- <u>Derivation of Schrödinger's Equation</u>
  - We derived

$$\hbar\omega = \frac{\hbar^2}{2m}\vec{k}^2 + V\left(\vec{r},t\right).$$

  - Assume that the wave equation we are looking for is <u>linear</u>. If this is the case, the solution can be written as <u>Fourier representation</u>

$$\Psi\left(\vec{r},t\right) \propto e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}.$$

  - Because of the reason discussed on the previous slide, we compute the first time-derivative

$$\frac{\partial\Psi}{\partial t} = \frac{\partial}{\partial t}e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)} = -i\omega\Psi.$$

  - Using the relation derived above gives us

$$i\hbar\frac{\partial\Psi}{\partial t} = \hbar\omega\Psi = \frac{\hbar^2}{2m}\vec{k}^2\Psi + V\left(\vec{r},t\right)\Psi.$$

Review of Quantum Mechanics I

- Derivation of Schrödinger's Equation
  - We derived

$$i\hbar\frac{\partial\Psi}{\partial t} = \hbar\omega\Psi = \frac{\hbar^2}{2m}\vec{k}^2\Psi + V\left(\vec{r},t\right)\Psi.$$

  - Consider the first term on the right-hand-side

$$\vec{k}^2\Psi = \vec{k}^2 e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)} = -\Delta e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)} = -\Delta\Psi.$$

  - Using this above yields

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V\left(\vec{r},t\right)\Psi.$$

  - This is the time-dependent Schrödinger equation.
  - It describes non-relativistic particles without spin.
  - It is a Partial Differential Equation (PDE)!

Review of Quantum Mechanics I

- Operators in Quantum Mechanics
  - The energy-momentum relation is given by

$$E = \frac{p^2}{2m} + V\left(\vec{r}, t\right).$$

  - Multiply this by the wave function to obtain

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi.$$

  - Replace the quantities E and p by the following operators

$$E \to \hat{E} = i\hbar\frac{\partial}{\partial t} \qquad \text{and} \qquad p_n \to \hat{p}_n = -i\hbar\frac{\partial}{\partial x_n}.$$

  - Using those formal replacements of classical quantities by the corresponding operators gives us

$$\hat{E}\Psi = \frac{\hat{p}^2}{2m}\Psi + V\Psi \quad \to \quad i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V\left(\vec{r}, t\right)\Psi.$$

Review of Quantum Mechanics I

- Normalization and Moments
  - Assume that we describe the bound state of a single particle. Then we require that the following normalization condition is satisfied

$$\int d^3r \; \Psi\left(\vec{r},t\right)\Psi^*\left(\vec{r},t\right) = 1.$$

  - Consider the time-independent one-dimensional case. Then we have

$$\Psi\left(\vec{r},t\right) = \Psi\left(x\right).$$

  - In this case the normalization condition becomes simply

$$\int_{-\infty}^{+\infty} dx \; \Psi\left(x\right)\Psi^*\left(x\right) = 1.$$

  - We define the *n*th moment via

$$\langle x^n \rangle = \int_{-\infty}^{+\infty} dx \; \Psi\left(x\right)x^n\Psi^*\left(x\right).$$

Review of Quantum Mechanics I

- <u>The Heisenberg Uncertainty Relation</u>
  - Consider a simple 1D Gaussian wave of the form

    $$\Psi(x) = \Psi_0 e^{-ax^2}.$$

  - Determine the constant Ψ_0 via the normalization condition

    $$\int_{-\infty}^{+\infty} dx\ \Psi(x)\Psi^*(x) = \Psi_0\Psi_0^* \int_{-\infty}^{+\infty} dx\ e^{-2ax^2} = 1.$$

  - By using the Gaussian integral

    $$\int_0^{\infty} dx\ e^{-bx^2} = \frac{\sqrt{\pi}}{2\sqrt{b}}$$

    we find

    $$\Psi_0\Psi_0^* \int_{-\infty}^{+\infty} dx\ e^{-2ax^2} = \Psi_0\Psi_0^* \sqrt{\frac{\pi}{2a}} = 1.$$

Review of Quantum Mechanics I

- <u>The Heisenberg Uncertainty Relation</u>
  - Therefore, we need

$$\Psi_0 \Psi_0^* = \sqrt{\frac{2a}{\pi}}.$$

  - The second moment is given by

$$\langle x^2 \rangle = \int_{-\infty}^{+\infty} dx\ \Psi(x) x^2 \Psi^*(x) = \Psi_0 \Psi_0^* \int_{-\infty}^{+\infty} dx\ x^2 e^{-2ax^2} = \frac{1}{4a}.$$

  - We use the Fourier transforms

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\ \Phi(k) e^{ikx},$$

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx\ \Psi(x) e^{-ikx}.$$

Review of Quantum Mechanics I

- <u>The Heisenberg Uncertainty Relation</u>
  - Compute the Fourier transform of the Gaussian

$$\Phi(k) = \frac{\Psi_0}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dx\; e^{-ax^2} e^{-ikx}$$

$$= \frac{\Psi_0}{\sqrt{2a}} e^{-k^2/(4a)}.$$

Is also a Gaussian!!!

  - Calculate the second moment in Fourier space

$$\langle k^2 \rangle = \int_{-\infty}^{+\infty} dk\; \Phi(k) k^2 \Phi^*(k)$$

$$= \frac{\Psi_0 \Psi_0^*}{2a} \int_{-\infty}^{+\infty} dk\; k^2 e^{-k^2/(2a)}$$

$$= a.$$

Review of Quantum Mechanics I

- <u>The Heisenberg Uncertainty Relation</u>
  - We derived for the two moments

$$\begin{aligned}\langle x^2\rangle &= \frac{1}{4a},\\ \langle k^2\rangle &= a.\end{aligned}$$

  - Therefore, we find for the product of the two second moments

$$\langle x^2\rangle\langle k^2\rangle = \frac{1}{4}.$$

This is a property of the Fourier transform!

  - Note that the widths of the two Gaussians are

$$\begin{aligned}\Delta x &= \sqrt{\langle x^2\rangle} = \frac{1}{2\sqrt{a}}\\ \Delta k &= \sqrt{\langle k^2\rangle} = \sqrt{a}.\end{aligned}$$

Review of Quantum Mechanics I

- The Heisenberg Uncertainty Relation
  - For the product of the two widths we, therefore, obtain

$$\Delta x \Delta k = \frac{1}{2}.$$

  - Using the de Broglie relation $p = \hbar k$ yields

$$\Delta x \Delta p = \frac{\hbar}{2}.$$

  - Note that this was derived for a Gaussian wave.
  - In general we have

$$\Delta x \Delta p \geq \frac{\hbar}{2}.$$

  - This is the famous uncertainty relation!
  - The proof will be discussed later.

Review of Quantum Mechanics I

- The Continuity Equation
  - Schrödinger's equation is given by

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + V\left(\vec{r},t\right)\Psi.$$

  - Its complex conjugate is

Assume a real potential

$$-i\hbar\frac{\partial\Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi^* + V\left(\vec{r},t\right)\Psi^*.$$

  - Remember that the probability density is $\Psi\Psi^*$.
  - The time-derivative of the probability density is

$$\frac{\partial}{\partial t}\Psi\Psi^* = \Psi\frac{\partial\Psi^*}{\partial t} + \Psi^*\frac{\partial\Psi}{\partial t}.$$

Use Schrödinger's equation

Review of Quantum Mechanics I

- <u>The Continuity Equation</u>
  - With the help of the Schrödinger equation we derive

$$\begin{aligned}\frac{\partial}{\partial t}\Psi\Psi^* &= \Psi\frac{\partial\Psi^*}{\partial t} + \Psi^*\frac{\partial\Psi}{\partial t} \\ &= \frac{\Psi}{-i\hbar}\left[-\frac{\hbar^2}{2m}\Delta\Psi^* + V\Psi^*\right] + \frac{\Psi^*}{i\hbar}\left[-\frac{\hbar^2}{2m}\Delta\Psi + V\Psi\right] \\ &= \frac{\hbar}{2im}\Psi\Delta\Psi^* - \frac{1}{i\hbar}V\Psi^*\Psi - \frac{\hbar}{2im}\Psi^*\Delta\Psi + \frac{1}{i\hbar}V\Psi\Psi^* \\ &= \frac{\hbar}{2im}\Big(\Psi\Delta\Psi^* - \Psi^*\Delta\Psi\Big).\end{aligned}$$

  - To rewrite this we consider the following (just product rule)

$$\begin{aligned}\vec{\nabla}\cdot\left(\Psi\vec{\nabla}\Psi^*\right) &= \vec{\nabla}\Psi\cdot\vec{\nabla}\Psi^* + \Psi\Delta\Psi^* \\ \vec{\nabla}\cdot\left(\Psi^*\vec{\nabla}\Psi\right) &= \vec{\nabla}\Psi^*\cdot\vec{\nabla}\Psi + \Psi^*\Delta\Psi.\end{aligned}$$

Subtract these two equations

Review of Quantum Mechanics I

- The Continuity Equation
  - By combining all this, we derive

$$\begin{aligned}\frac{\partial}{\partial t}\Psi\Psi^* &= \frac{\hbar}{2im}\Big(\Psi\Delta\Psi^* - \Psi^*\Delta\Psi\Big)\\ &= -\vec{\nabla}\cdot\left[\frac{\hbar}{2im}\Big(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\Big)\right].\end{aligned}$$

  - For the probability density we can use $\rho=\Psi\Psi^*$.
  - Furthermore, we define the particle current density via

$$\vec{j} := \frac{\hbar}{2im}\Big(\Psi^*\vec{\nabla}\Psi - \Psi\vec{\nabla}\Psi^*\Big).$$

  - Using this above yields

$$\frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{j} = 0.$$

This is a typical continuity equation.

Review of Quantum Mechanics I

- The Continuity Equation
  - We found the continuity equation

$$\frac{\partial}{\partial t}\rho + \vec{\nabla} \cdot \vec{j} = 0.$$

  - Integrating this over the volume V yields

$$\int_V d^3r \, \frac{\partial \rho}{\partial t} = -\int_V d^3r \, \vec{\nabla} \cdot \vec{j}.$$

  - We rewrite the left-hand-side and for the right-hand-side we use the divergence theorem to derive

$$\frac{d}{dt}\int_V d^3r \, \rho = -\int_{\partial V} d\vec{S} \cdot \vec{j}.$$

Describes conservation of particles!

Number of particles in V

Particle flux through surface of the volume V