

Computational
Journey of

Quantum Mechanics



Preface

Welcome, fellow explorers of quantum mechanics!

If you're reading this, chances are you're diving into the depths of quantum mechanics and looking for a way to bridge the gap between abstract theory and practical implementation. This course is designed to be that bridge, transforming complex quantum concepts into computational models, algorithms, and visualizations. By the end of this journey, you'll not only understand quantum mechanics theoretically but also be comfortable implementing its principles computationally.

Like it or not, computers play a key role in our understanding of the universe. They help us analyze immense datasets, maintain accuracy in simulations, and provide faster solutions to problems that would take weeks to solve manually. That is why this course exists. Through a structured series of Mathematica notebooks, we will explore quantum mechanics while focusing on code development and algorithmic implementation. Each notebook will combine theoretical explanations with executable code, hands-on exercises, and visualization techniques to reinforce learning.

Here, we will take what you learn in class and apply it computationally—developing numerical techniques, symbolic calculations, and simulations to gain deeper insight into quantum phenomena. Each week, I will provide Mathematica notebooks, and we will have video discussions or local gatherings to clarify concepts, troubleshoot code, and explore advanced topics together.

This course will take you through the fundamentals of scientific computing, computational quantum mechanics, wave mechanics, quantum dynamics, and advanced topics such as quantum chaos, quantum information, and quantum technologies. Whether your goal is research, quantum computing, or a strong computational foundation in physics, this course will equip you with the skills to succeed.

So, let's get started! Bring your curiosity, your questions, and your willingness to experiment—because in quantum mechanics, as in life, the most profound insights often come from unexpected places.

Our Goals and Considerations

This course is meticulously structured to transform your theoretical understanding into practical computational skills. We will bridge the gap between abstract quantum theory and concrete numerical and symbolic implementation, equipping you with the tools to simulate and visualize quantum phenomena across multiple domains.

Learning Approach

Each week, we will explore theoretical concepts and implement them through Mathematica notebooks. Our learning strategy will emphasize:

- > Clear, executable code examples.
- > Visualization of quantum phenomena.
- > Incremental skill development.
- > Connections between theory and computation.
- > Open-ended exploration opportunities.

Outline

Volume 0: Fundamentals of Scientific Computation

Before diving into quantum mechanics, we will establish a strong computational foundation. This volume introduces essential numerical and symbolic methods, including floating-point arithmetic, numerical differentiation and integration, differential

equations, optimization techniques, and visualization fundamentals. While this volume can be skipped by students familiar with computational methods, it serves as a valuable reference for those needing a refresher.

Volume 1: Foundations of Computational Quantum Mechanics

We begin our quantum journey with the mathematical formalism of quantum mechanics. Topics include quantum state representation, operator algebra, linear algebra techniques for quantum systems, and computational methods to analyze quantum behavior. By the end of this volume, you will have a robust computational framework for exploring quantum phenomena through simulation and visualization.

Volume 2: Quantum Dynamics, and Simulation

This volume delves into time evolution in quantum mechanics, wave packet dynamics, and numerical approaches to solving the Schrödinger equation. You will gain intuition for quantum motion through computational studies of the harmonic oscillator, Ehrenfest's theorem, and phase space representations.

Volume 3: Advanced Quantum Mechanical Systems

Building on earlier volumes, we explore angular momentum, spin systems, perturbation theory, and quantum tunneling. Through numerical and symbolic methods, we will simulate spin precession, study the effects of spin-orbit coupling, and implement approximation techniques used in advanced quantum mechanics.

Volume 4: Complex Quantum Systems

This volume extends computational techniques to more sophisticated quantum systems, including the hydrogen atom, relativistic quantum mechanics, and scattering theory. Topics include numerical solutions to central potential problems, Dirac equation simulations, and computational approaches to quantum scattering.

Volume 5: Frontier Topics in Computational Quantum Mechanics

Here, we venture into cutting-edge computational quantum physics. Topics include quantum chaos, open quantum systems, tensor network methods, and Monte Carlo simulations for many-body quantum mechanics. This volume introduces techniques used in modern research and state-of-the-art quantum simulations.

Volume 6: Quantum Technologies

In the final part of the course, we explore practical applications of quantum mechanics in emerging technologies. Topics include quantum computing, quantum information processing, molecular quantum mechanics, and high-performance computing for quantum simulations. You will implement fundamental quantum algorithms, error correction techniques, and quantum-inspired machine learning approaches.

Weekly Deliverables

Every week, I will provide Mathematica notebooks covering topics of discussion. These notebooks will include:

- > *Theoretical Explanations*: Background concepts necessary for understanding the computational approach.
- > *Executable Code*: Fully functional code snippets that implement the key ideas.
- > *Exploratory Exercises*: Open-ended problems encouraging you to experiment and deepen your understanding.

Additionally, we will have video discussions or local gatherings where you can ask questions, clarify doubts, and discuss implementations. This interactive approach ensures that you not only learn quantum mechanics computationally but also gain hands-on experience in applying these techniques.

FAQ

Q : Do I need prior programming experience?

A : Some familiarity with coding, particularly in Mathematica, is helpful but not required . We will cover essential programming concepts as needed.

Q : How will I receive the notebooks and materials?

A : Weekly Mathematica notebooks will be shared online via ELearn, and on my personal github, and you' ll have access to them for reference and practice .

Q : How can I ask questions or seek help?

A : We will have weekly discussions, and you can also reach out via email or during local gatherings.

About Me

My name is Amir, and I'm a physics student at university of Tehran. I am also a software developer. My experience spans from numerical relativity, to writing front-end and designing user interfaces. I also care about open-source, freedom of knowledge, and decentralization of academia. My life-long project is *Independent Society of Knowledge* and it is embodiment of the things I love to see in scientific community. For contacting me:

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If you have any questions, feel free to reach out. I look forward to embarking on this quantum computational journey with you!