Quantum Chemistry Course Introduction

CHEM 361B: Introduction to Physical Chemistry

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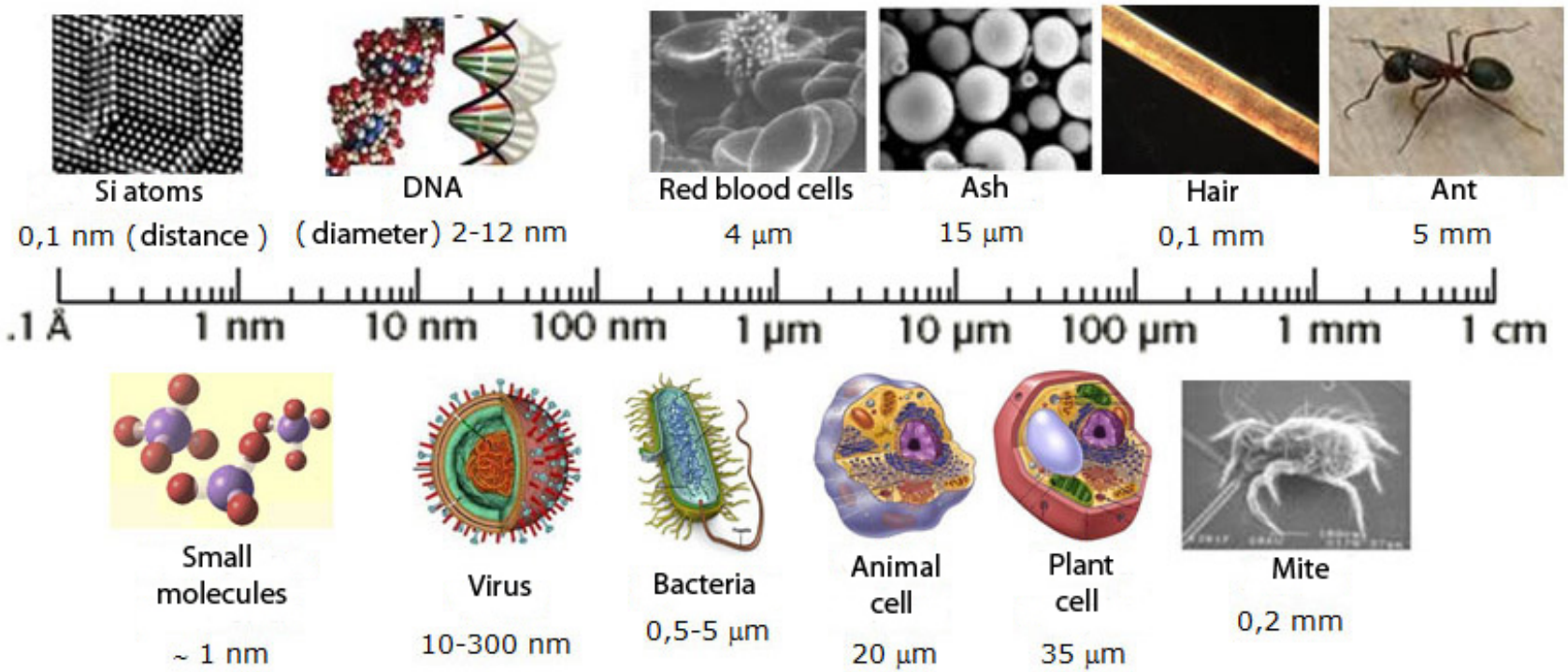
Lecture 0

What is Quantum Mechanics?

Quantum Mechanics: A theory that predicts the properties of particles at the atomic and sub-atomic scale

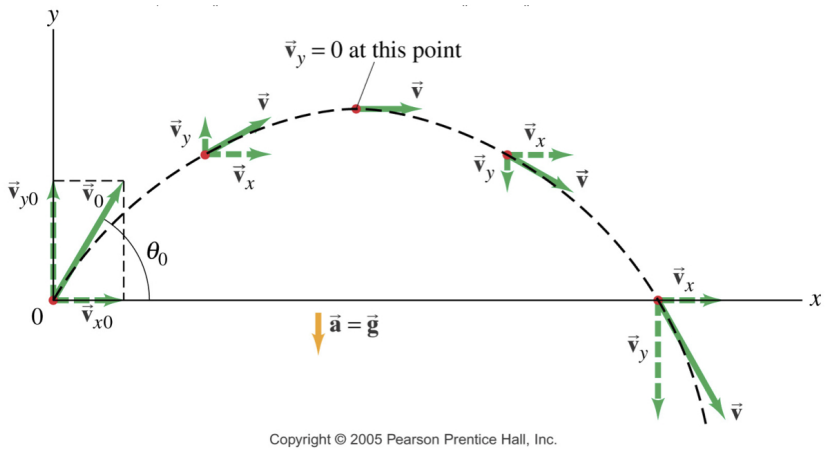


Quantum Mechanics
Probabilistic

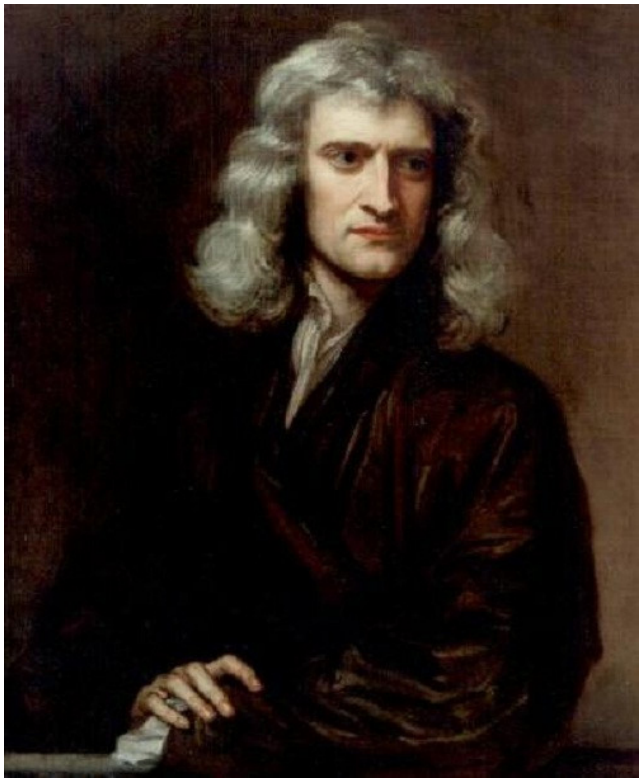
Classical Mechanics
Deterministic

Classical Mechanics - The Future Is Known

Deterministic System: A system in which no randomness is involved in the development of future states of the system



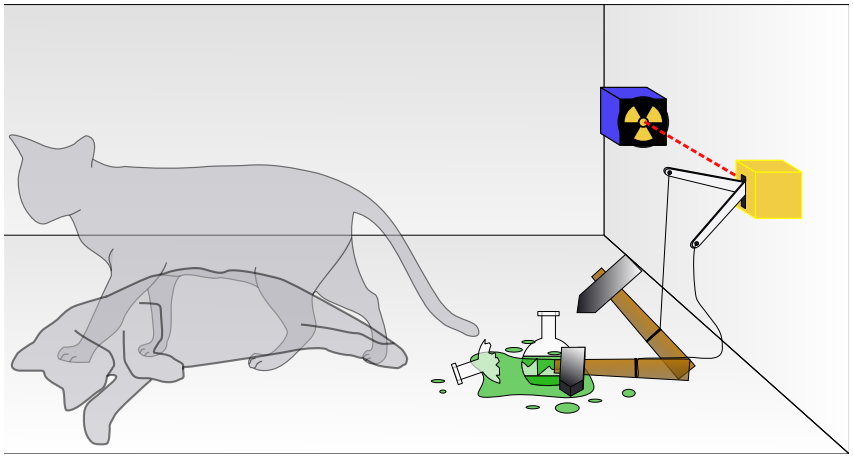
Can predict with certainty the state of an object for all time.



Sir Issac Newton (1643-1727)

Quantum Mechanics - Probabilities Reign Supreme

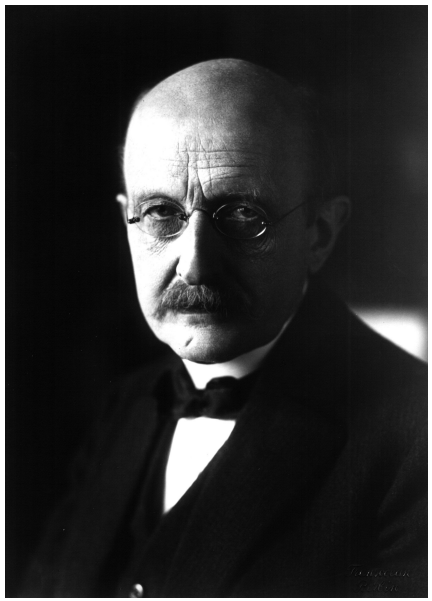
Probabilistic System: A system where the occurrence of events cannot be perfectly predicted. The behavior of such a system can be described in terms of probability.



Schrödinger's Cat thought experiment

By Dhatfield - Own work, CC BY-SA 3.0,

https://commons.wikimedia.org/w/index.php?curid=4279886

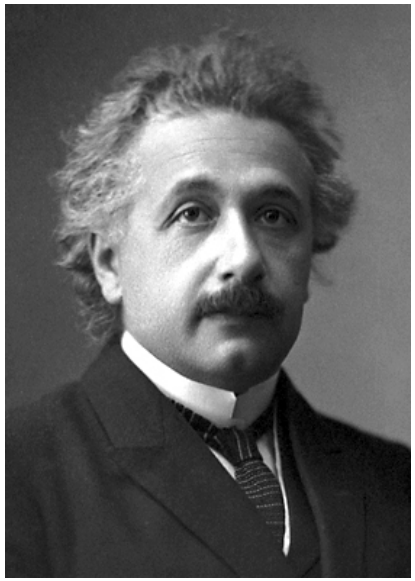


Max Planck (1858-1949)

Thoughts about Quantum Mechanics

Quantum Mechanics is not intuitive!

Richard Feynman: 'If you think you understand quantum theory . . . you don't understand quantum theory.'



Albert Einstein: 'God does not play dice with the universe.'

Do not try to rationalise Quantum Mechanics from your deterministic point of view. Instead, focus on learning how to use the theory to make predictions about atomic systems.

Course Learning Objectives

The course learning objectives are

1. Develop an understanding of the nature of quantum systems and apply these principles to solve the Schrödinger Equation and determine physical observables.
2. Understand what it means for a system to be quantized and relate the quantized nature of energy from the Schrödinger Equation to predict spectroscopic phenomena including: electronic, vibrational, NMR, and rotational spectroscopy.
3. Use the solutions to the Schrödinger Equation to describe how chemical bonds are formed between atoms.

Teaching Philosophy

1. Flipped classroom and active learning
2. In evaluations demonstrate your knowledge
3. During the semester, you are allowed to have a bad day
4. If you think there is a problem with how I evaluated you, ask
5. All grades are posted to TITANium. What is posted there will be your final grade
6. This is not a calculus course, but you are expected to be able to use it
7. Questions regarding course content will most likely be answered on the course discussion board

Summary

- Quantum mechanics is a probabilistic theory that is best applied to atomic systems
- We will use it to make predictions regarding spectroscopy and the nature of bonding between atoms
- Do not try to rationalize the theory. Instead, focus on learning how to use the theory to make predictions about atomic systems.