



Module PMRF- ISSS057/2023

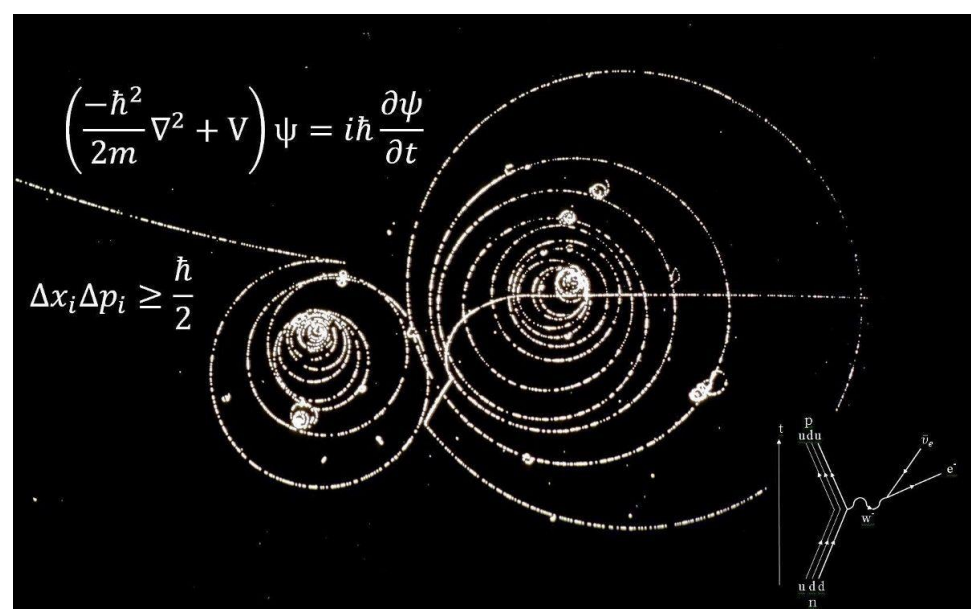
Computational Methods for Quantum Systems

Name of the PMRF student

Asif Altaf Shah

Required background of the students

- PG/ final year UG students from engineering and science background.



If you aren't confused by quantum mechanics, you haven't really understood it.

Neils Bohr

Details of the content of the module

This course will focus on Computational approaches for solving Quantum Systems. The broader context of topics will include introduction to non-interacting, interacting quantum systems in the framework of Density Functional Theory & their application to solids.

1. Schrödinger equation, N electrons & Born-Oppenheimer approximation.
2. Variational principle - The blind Man's stick.
3. Hartree, Hartree-Fock Methods.
4. Introduction to Density Functional Theory (DFT).
5. Mathematical Functionals & Kohn-Sham theorems.
6. Correlation Energy- The unknown piece of puzzle.
7. Estimating XC functionals- The beginning of trade offs.
8. Density Functional Theory for solids.
9. Quantum packages- ATK, VASP, Espresso etc

Schedule of the module

Start Date: Sunday, 29 October 2023

Occurrence: Every Sunday

Lecture Duration: 1-1.5 hours

Total lectures- 40 to 50

Meeting link : Will be shared later

Contact email ID: asifshah@iisc.ac.in

Registration link:

https://docs.google.com/forms/d/e/1FAIpQLSe7rUklqOypAywFMcFDuUf6ZnNQRNiEf_rkK_Yi7S9LEEOzkuQ/viewform?usp=sf_link