Approved in 50th BoA Meeting(14.07.2023)

IIT Mandi
Proposal for a New Course

Course number **: PH608**
Course Name **: Computer assisted quantum mechanics**
Credit Distribution : *2-0-3-3*
Intended for **:** UG/PG/I-PhD/PhD elective
Prerequisite : PH301/PH513 (Quantum Mechanics), PH524/EP403 (Physics of Atoms and Molecules), PH613 (Computational methods for physicists)/EP302 (Computational methods for engineering)
Mutual Exclusion : NA

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1. Preamble:

The objective of this course is to provide an introduction to some of the basic computational techniques used in quantum mechanics. It mainly teaches how to numerically solve Schrodinger equations (both time-independent and time-dependent). It starts with single particle systems and later deals with the many-electron systems. Students have to implement all the methods during the lab sessions using Fortran/C/Python for the specific quantum mechanical problems given. These exercises provide deep insights to some the computational aspects used in quantum mechanics particularly in the field of atomic/molecular/condensed matter physics.

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The hours mentioned below include lecture and lab sessions

2. Course Modules with quantitative lecture hours:

Module1: The single-particle problem- Time independent Schrodinger equation and its solution with Numerov's method, Bound state solutions for one-dimensional (1D) case such as Harmonic oscillator, Schrodinger equation for central potentials, solutions of hydrogen atom, scattering from different type of central potentials, Response of atoms to external fields

(20 hours)

Module 2: Variational method-The variational principle, Numerical solutions to quantum mechanical problems using variational methods, Plane-wave basis set and Non-orthonormal basis set

(15 hours)

Module 3: Multi-electron systems-Basics of Hartree-Fock (HF) methods and its numerical implementation to a few selected problems, going beyond HF methods, density functional theory and its implementation with some specific examples for simple atomic

systems.

(15 hours)

Module 4: Time propagation- Spectral methods, direct numerical integration, split operator and Crank-Nicolson methods. Implementation of these methods to a few quantum mechanical systems

(20 hours)

3. Text books:

1) Computational Physics by J. M. Thijssen (Cambridge University Press, 2007)
2) Computational Quantum Mechanics by J. Izaac and J. Wang (Springer, 2018)

4. References:

1) **Numerical methods in quantum mechanics by** Paolo Giannozzi (Online lecture notes, http://www.fisica.uniud.it/~giannozz/Corsi/MQ/LectureNotes/mq.pdf)
2) **Computational physics,** R. H. Landau, M. J. Páez and C. C. Bordeianu (2015 WILEY-VCH Verlag)

5. Similarity with the existing courses: NA

(Similarity content is declared as per the number of lecture hours on similar topics)

6. Justification of new course proposal if cumulative similarity content is >30%:

NA