CHM 667A
Quantum Dynamics in Chemistry

First course handout

Mainak Sadhukhan

Indian Institute of Technology Kanpur

Topics to be covered

- Recapitulations of basic concepts of Quantum Mechanics
- Approximation methods: Time-dependent Perturbation Theory and Dirac-Frenkel variational method with applications in reaction dynamics.
- Statistical perspectives of quantum dynamics for composite quantum systems
- Density matrix theories for open quantum systems
- The path integral approach and its applications in chemistry
- Introduction to relativistic quantum mechanics.
- Trajectory picture of quantum dynamics
- **Applications:** • Chemical Dynamics theory • Radiation-matter interaction • Matters under strong external fields: Attosecond spectroscopy [1]

[1] Red coloured topics were part of the course had the time permitted.

Grading policy

- One in-course micro-project presentations (50 marks each)
- Assignments may be given for practice only
- Final marks and grades will be prorated based on the micro-project.

References

Books

1. Quantum Mechanics, Albert Messiah
2. Modern Quantum Mechanics, J. J. Sakurai
3. Quantum Dynamics, E. Bittner
4. Quantum Mechanics, E. Merzbacher
5. Quantum Mechanics and path integrals, R. P. Feynman and A. R. Hibbs

Online resources

Anything - but with an implied caution for authenticity and correctness!

Contact informations

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