PHYS 5393/6393
Syllabus

Elements of Quantum Energy and Information Transfer

CRN: 17403,17404
Term: Fall 2024
Prerequisite: PHYS 4355 or equivalent

Course hours: M,W at 4:30 PM - 6:30 PM Mountain Time

Location: PSCI 218 or 320

Instructors: T. Baruah, K. A. Jackson(external), M. R. Pederson, Y-P. Shim

Offices: PSCI 120 (Baruah)

PSCI 209 (Pederson)

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Office hours:
Baruah TR(10:00 - 11:00 am) or by appointment
Pederson MW (After Class) or by appointment
Shim MW (After Class) or by appointment

Course Description and Objectives:

This course will provide the students with a brief introduction to density functional theory (DFT) and its applications to molecular systems. The students will learn to perform DFT calculations using the NRL-MOL/FLOSIC software. The students will learn to use the software to understand the structure-property relations, difference between closed and open shell systems, magnetic properties and to determine parameters for model Hamiltonians. They will also learn about self-interaction errors in density functional approximations (DFA) and self-interaction correction (SIC) using the FLOSIC method. In the latter part of the course, students will learn about quantum two-level systems and how to manipulate such systems, which is the foundation of quantum computing.

Upon completion of the course, the student should
a) be able to run calculations in a standard linux environment using the available queuing system, in the AQE, and on their laptops
b) be able to calculate the ground state properties of molecular systems with and without SIC
c) Determine parameters from DFT calculations for model Hamiltonians including magnetic systems
d) Perform analysis of the quantum behavior (energy and information transfer) of such systems
e) Understand how to control quantum two-level systems such as qubits.

Communication

The main communication methods are:
a) Classroom announcements and emails
b) Overleaf document for assignments and other materials
c) Blackboard announcement

Grading Policy:

- Attendance and Quizzes: 20%
- Final report: 20%
- Final presentation: 30%
- Assignments: 30%

Assignments

Assignments will be posted on overleaf and/or Blackboard on a weekly basis.

1. Amplitude Oscillations in Stark Effects
   (a) 2s Hydrogen atom exposed to a sudden electric field (BOE)
   (b) Neon in 3s excited exposed to a sudden electric field (NRLMOL)
2. Foerster Resonance
   (a) Two dipole carrying harmonic oscillators.
   (b) C_6 vdW calculation for Ne, Ar, Kr
   (c) C_6 vdW calculation for molecules
3. Quantum Tunneling
   (a) The Quantum Garage
   (b) The Spin on a Ring
   (c) $Mn_{12} - Acetate$
4. Spin-Spin Interactions
   (a) Singlet-Triplet Fission
   (b) Two Spin-Polarized ($H^{up} - He - H^{dn}$)
5. Controlling Qubit Systems
   (a) Rabi oscillation
   (b) Two-qubit system with non-Heisenberg exchange interaction

Technology Requirements

You can use the computers in PSCI 218 or bring your own personal laptop. Access to computational platforms and software for running the programs will be provided to the students.

IMPORTANT: If you encounter technical difficulties beyond your scope of troubleshooting, please contact the UTEP Help Desk (https://www.utep.edu/technologysupport/) as they are trained specifically in assisting with the technological needs of students. Please do not contact me for this type of assistance. The Help Desk is much better equipped than I am to assist you!

Course Policies

Students with Disabilities:

If you have a disability and need classroom accommodations, please contact The Center for Accommodations and Support Services (CASS) at 747-5148, or by email to cass@utep.edu, or visit their office located in UTEP Union East, Room 106. For additional information, please visit the CASS website at https://www.utep.edu/student-affairs/cass/. Accommodations might include but are not limited to note takers, readers, or extended time on exams and assignments. Please take care of this as soon as possible and before the first exam.

Scholastic Integrity:

Academic dishonesty is prohibited and is considered a violation of the UTEP Handbook of Operating Procedures. It includes, but is not limited to, cheating, plagiarism, and collusion. Cheating may involve copying from or providing information to another student, possessing unauthorized materials during a test, or falsifying research data on laboratory reports. Plagiarism occurs when someone intentionally or knowingly represents the words or ideas of another as ones' own. Collusion involves collaborating with another person to commit any academically dishonest act. Any act of academic dishonesty attempted by a UTEP student is unacceptable and will not be tolerated. All suspected violations of academic integrity at The University of Texas at El Paso must be reported to the Office of Student Conduct and Conflict Resolution (OSCCR) for possible disciplinary action. To learn more, please visit HOOP: Student Conduct and Discipline.

Weekly Schedule

This is the weekly schedule we plan to follow. The students are encouraged to form groups with one experienced user per group.
Week 1 : Introduction to Linux commands, vi editor, compilation and job submission protocols; introduction to quantum oscillation
Week 2 : *Basic electronic structure of atoms and molecules* . Introduction to DFT. NRLMOL input & output files
Week 3 : Geometry optimization, structure property relations
Week 4 : Introduction to FLOSIC; PNNL talk.
Week 5 : Vibrational modes
Week 6 : *Dipoles, electric fields, and polarizability*
Week 7 : *Spin and magnetism in molecules I*
Week 8 : *Spin and magnetism in molecules II*
Week 9 : *DFT and chemistry: reaction energies and reaction barriers*
Week 10 : Electron-phonon coupling
Week 11 : (Shim) Introduction to Python and Jupyter Notebook
Week 12 : (Shim) Quantum two-level system
Week 13 : (Shim) Jaynes-Cummings model
Week 14 : (Shim) Exchange interaction between two spins
Week 15 : Student final presentations