Ankit Mahajan

Contact Information

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Research Interests

I am interested in **condensed matter physics** and **quantum chemistry**, specifically in computational electronic structure theory. My other interests include nonlinear dynamics and quantum computing.

Education

Indian Institute of Technology, Bombay (IITB), Mumbai, India

5 Year Integrated MSc in Physics — *July 2012 - April 2017 (Expected)*
(converted from BTech Engineering Physics in *July, 2015*)
Minor in Computer Science and Engineering
Cumulative Performance Index: **8.92** on 10

Test Scores

General GRE: **334/340** (Verbal: 164/170, Quantitative: 170/170, Writing: 4.0/6.0)
Physics GRE: **990/990**
TOEFL: **111/120** (Reading: 30/30, Listening: 28/30, Speaking: 26/30, Writing: 27/30)

Research Experience†

Master's Thesis: *Ab initio* molecular dynamics using fragment-based electronic structure theory — *July, 2016 - Ongoing*
Guide: Prof. Srinivasan Iyengar, Indiana University, Bloomington
Co-guide: Prof. Aftab Alam, IIT Bombay
I am studying the applications of a fragment-based electronic structure method, PIE-ONIOM, to *ab initio* molecular dynamics. I have learned about two composite quantum chemical approaches, *viz.* hybrid methods (QM/MM, ONIOM) and fragment-based methods (FMO, MTA), through a literature survey. I have modified the existing PIE-ONIOM wrapper code to allow combinations of different electronic structure packages. Our goal is to study the applicability of DMRG within the PIE-ONIOM approach for both static and dynamics calculations.

BTech Project: DMRG calculations of π-conjugated oligomers within the Pariser-Parr-Pople model — *July, 2015 - July, 2016*
Guide: Prof. Alok Shukla, IIT Bombay
In the first phase, I studied the basics of electronic structure theory including plane wave methods, tight binding, HF, CI, etc. in the second quantized formalism. In the second phase, I learned the theory of Density Matrix Renormalization Group using Matrix Product States. We did benchmark DMRG-CI calculations of $\pi-$conjugated oligomers (t-PA, polyacenes, PPP, trigonal quantum dots) starting with the HF orbitals of the Parriser-Parr-Pople Hamiltonian. The DMRG-CI energies were found to compare favorably FCI, QCI and MRSDCI results, wherever applicable. A publication based on these results is under preparation.

Summer Internship: Quantum Wavepacket *Ab Initio* Molecular Dynamics (QWAIMD) on an adaptive, moving grid — *Summer 2015*
Guide: Prof. Srinivasan Iyengar, Indiana University, Bloomington
I studied various techniques of *on-the-fly ab initio* molecular dynamics, with focus on Atom Centered Density Matrix Propagation. I learned about the hydrodynamical formulation of quantum dynamics (Bohmian mechanics). QWAIMD treats one nucleus in the system quantum mechanically by propagating a wave-packet on a grid. We worked out the theory of a grid moving with the

wave-packet using Pulay forces. I was able to modify the QWAIMD `FORTRAN` code to implement an adaptive, vibrating grid using Distributed Approximating Functionals (DAF).

Supervised Learning Project: Simulating the response of a Hodgkin-Huxley neuron cable to an external electromagnetic field *July, 2014 - November, 2014*
Guide: Prof. Punit Parmananda, IIT Bombay
I learned about the Fitzhugh-Nagumo and Hodgkin-Huxley models of neuronal activity. We modified the HH cable equations, a set of four coupled, nonlinear partial differential equations, to include the effects of a time dependent EM field. The system was numerically integrated using `MATLAB`. We found that certain frequencies of the EM field can elicit an action potential response. Presence of an Arnold tongue in the forcing amplitude-frequency parameter space was demonstrated.

Paper in Preparation†

A paper titled **DMRG calculations of π-conjugated oligomers within the Pariser-Parr-Pople model** is under preparation in collaboration with Prof. Alok Shukla.

Key Course Projects†

Gauge kinematics of deformable bodies *Spring 2015*
Guide: Prof. Ravi Banavar, IIT Bombay
Course: Differential geometric methods in control
I reviewed the paper, similarly titled, authored by Wilczek and Shapere. I studied the concepts of connections and parallel transport on principal fiber bundles. These structures, which provide a natural setting for describing dynamics of everyday deformable objects (a falling cat, for example), are ubiquitous in the gauge theories fundamental physical interactions. This problem provides a clearer view of the concepts involved compared to the abstract formulations of fundamental physical laws.

Superconductivity as a broken $U(1)_{EM}$ symmetry *Spring 2015*
Guide: Prof. Urjit Yajnik, IIT Bombay
Course: Special topics in particle physics (Advanced QFT)
I learned how gauge symmetries arise in the formulation of fundamental interactions and lend them a geometric meaning. I examined the Goldstone theorem and the way Higgs mechanism solves the problem of gauge field masses. I also studied how the spontaneous breaking of electromagnetic $U(1)$ gauge symmetry of the Ginzburg-Landau Hamiltonian can be used to explain the exotic properties exhibited by superconductors, like Meissner effect, flux quantization, etc.

Frequency analysis of audio signals (in a group of 3) *Autumn 2014*
Guide: Prof. Pradeep Sarin, IIT Bombay
Course: Microprocessor and digital electronics lab
We designed a real-time audio frequency analyzer using the ATMEGA microcontroller. Mic output was amplified using an opamp circuit and connected to the MCU. A fast Fourier transform of the discretized signal would be carried out and displayed on a screen in real time (functional for frequencies up to 28 kHz).

Movie database web application (in a group of 2) *Autumn 2014*
Guide: Prof. Umesh Bellur, IIT Bombay
Course: Database and information systems
We designed a web-enabled movie database based on the MVC architecture. The *model* part consisted of a Java application connected to a MySQL database through the JDBC API. JSP's were used for the *view*, to create dynamic web pages, and Java servlets worked as *controllers*. Functionalities implemented included listing all the movies starring an actor, awards won by a movie, etc.

† Reports and additional details can be found on my homepage.

Teaching Experience

Teaching Assistant
My duties as a TA included conducting weekly hour-long tutorials for resolving theory doubts and solving problems. I also helped in preparing and grading examination papers.

- Tutor of 48 UG freshmen for MA 105, Calculus *Autumn 2016*
- Tutor of 48 UG freshmen for PH 108, Basics of Electricity and Magnetism *Spring 2017*

Scholastic Achievements

- **Department rank 4** out of 43 Engineering Physics students before converting to integrated MSc.
- One of only two students to receive the top grade in the graduate level course *Nonlinear Dynamics*, one of three in *Quantum Computing*, *Lie Groups and Lie Algebras* and *Differential Geometric Methods in Control*.
- Awarded the KPMG scholarship 2013, to cover tuition expenses for a year, based on excellent academic performance in freshman year.
- Secured **All India Rank 931** in IIT Joint Entrance Examination (JEE) 2012 among about 500,000 candidates.
- Secured **State Rank 33** and **All India Rank 406** in All India Entrance Examination (AIEEE) 2012 among over 1 million candidates.
- Qualified for Kishore Vaigyanik Protsahan Yojana (KVPY) 2012 fellowship by Department of Science and Technology, Govt. of India.
- One among top 1000 students nationwide to be awarded the National Talent Search Examination (NTSE) 2012 scholarship by Govt. of India.

Technical Skills

- Programming languages: Extensive use of C/C++, Fortran, BASH, TCSH, MATLAB. Some experience with Java, Python, Mathematica, MySQL.
- Quantum Chemistry Packages: Gaussian, Psi4, Orca, Gamess UK, Tinker, Molden, VMD
- Web: HTML, CSS, JS, JSP
- Software packages: LaTeX 2_ε, Autocad, MS Office, Arduino IDE
- Operating Systems: Unix/Linux, Windows

References

- **Prof. Srinivasan Iyengar** (Senior thesis and summer internship guide)
  Department of Chemistry, Indiana University, 800 E Kirkwood Ave, Bloomington, IN 47405, United States
  Phone: +1 812 856 1875
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- **Prof. Alok Shukla** (BTech project guide and course instructor)
  Department of Physics, IIT Bombay, Powai, Mumbai 400076, India
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- **Prof. Aftab Alam** (Project guide and course instructor)
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