Khalid Hossain

Leadership Computing Facility, Argonne National Laboratory

Skills

- **5+** years of experience of developing **quantum simulation software** using denisty functional theory (**DFT**) with **python**.
- High performance computing **(HPC)** techniques (user level) to perform one of the largest simulations of the dynamics in fermionic systems using **wslda-toolkit**.
- Understanding of **superfluidity** (advanced) and **superconductivity** (intermediate) at both **phenomenological** and **microscopic** theory level.
- **Machine learning (ML)** techniques in calculating fission properties for nuclei using **PyTorch**.
- Comfortable using **energy optimization** techniques to determine initial states in superfluid systems.

Research Experiences

Postdoctoral Appointee January 2023 - Current
Supervisor: Corey Adams
Mentor: Kyle Felker
Leadership Computing Facility, Argonne National Laboratory

- *Deep Learning in Many-body Physics*
  We are working on calculating different ground state properties like density of nucleons in small to medium sized nuclei employing artificial neural network (ANN) based representation of the many-body wavefunction, and variational Monte-Carlo technique. The state-of-the- art calculations compute properties of nuclei up to total 6 nucleons. Our goal is to extend these simulations using distributed computing and leadership class facilities for larger systems (up to 20), providing us with insights into the fundamental nuclear interactions.
- *Performance Analysis of Supercomputing Applications*
  Our aim is to develop performance metrics and analyze them for scientific applications at different levels of distributed computing (single vs. multiple GPUs, nodes; medium to large scale distribution etc.) across many available hardware platforms like Intel, Nvidia, AMD etc. This will allow us to develop better programming strategies to operate leadership class supercomputers near the peak performance level.

Summer Intern June 2021 - August 2021
Supervisors: Marc Verriere, Irene Kim, and Nicolas Schunck
Nuclear Data and Theory Group, Lawrence-Livermore National Laboratory

- *Machine learning in nuclear theory*
  We are using machine learning techniques to determine nuclei's ground state and fission properties across the nuclear chart. The project involves training a deep neural network (more precisely, a convolutional denoising autoencoder) to determine the Hartree-Fock-Bogoliubov solution from the first iterations of HFBTHO, a FORTRAN nuclear Density Functional Theory code actively developed in the Nuclear Data Group of LLNL. A properly trained network could drastically reduce the number of iterations to obtain self-consistent solutions of the HFB equations. The neural network is conceived and trained using the python library PyTorch.

Research Assistant May 2016 - May 2022
Supervisor: Michael McNeil Forbes, Ph.D.
Department of Physics and Astronomy, WSU, Pullman, WA

- *'Negative-mass' hydrodynamics*
  DFT implementation to simulate the dynamics of trapped ^{87}Rb Bose-Einstein condensate. This research led to the identification of the mechanism behind the origin of effective mass and explained observed phenomena in this bosonic superfluid system. In collaboration with the 'Fundamental Quantum Physics' lab of Professor Peter Engels at Washington State University.
- *Andreev-Bashkin effect (entrainment, dissipationless superfluid drag)*
  Developed an experimental protocol to directly detect bulk 3D entrainment in the superfluid mixture of ^{174}Yb (boson) and ^{6}Li (fermion). Entrainment has been predicted by A. F. Andreev and E. P. Bashkin in 1975 and has

not been experimentally observed ever since. The experimental detection is expected to shed light on the long-standing astrophysical mystery of neutron star 'glitch' – a sudden increase in the rotation rate of the star. Entrainment is believed to play a crucial in the development of this effect. This research is done in close collaboration with Professor Subhadeep Gupta's lab at University of Washington.

- *Rotating Quantum Turbulence*
  Quantum turbulence is characterized by the dynamic interactions between quantized vortices in superfluids. We are developing orbital-free DFT models to study these interactions in a rotating system and validate the results against more accurate TDDFT models like superfluid local density approximation (SLDA). This validation is crucial to build orbital-free density functionals to simulate the dynamics in macroscopically large samples of fermionic superfluids as time evolution of many orbitals for long times can be quite expensive numerically. This research is done in collaboration with Professor Gabriel Wlazłowski's group at Warsaw University of Technology, Poland.

- *Isotropic Quantum Turbulence*
  In similar spirit to the rotating turbulence project, but performed for isotropic superfluid in a 3D box. Involves handling of much larger data sets and HPC. Computing assignments and analysis will be performed in SUMMIT and RHEA – flagship supercomputing facilities maintained by Oak Ridge National Lab.

Education

- WASHINGTON STATE UNIVERSITY — Aug 2014 - May 2022
  Department of Physics and Astronomy, Pullman, WA
  Ph.D. in Atomic Physics
  Advisor: Michael McNeil Forbes, Ph.D.

- UNIVERSITY OF DHAKA — Jan 2012 - July 2013
  Dhaka, Bangladesh
  Master of Science in Theoretical Physics

Publications

- "Negative-Mass Hydrodynamics in a Spin-Orbit-Coupled Bose-Einstein Condensate"
  M. A. Khamehchi, **K.H.**, M. E. Mossman, Y. Zhang, Th. Busch, M. M. Forbes, and P. Engels.
  Phys. Rev. Lett. **118**, 155301 (2017)

- "Rotating Quantum Turbulence in the Unitary Fermi Gas"
  K.H., K. Kobuszewski, M. M. Forbes, P. Magierski, K. Sekizawa, and G. Wlazłowski.
  Phys. Rev. A **105**, 013304 (2021)

- "Detecting Entrainment in Fermi-Bose Mixture"
  K.H., S. Gupta, and M. M. Forbes.
  Phys. Rev. A **105**, 063315 (2022)

Talks

- "Homogeneous and Isotropic Turbulence across the BEC-BCS Crossover "
  APS DAMOP Virtual Meeting — June, 2021

- "Quantum Turbulence: Generation and Decay in Bosonic and Fermionic Superfluids"
  APS DAMOP Virtual Meeting — June, 2020

- "Energy Dissipation and Vortex Recombination in the Unitary Fermi Gas"
  APS DAMOP meeting — May, 2019

- "Detecting Entrainment in Fermi-Bose Mixtures"
  APS DAMOP meeting — May, 2018

- "Negative-mass Hydrodynamics in a spin-orbit coupled Bose-Einstein Condensate"
  APS DAMOP meeting — June 2017

Awards and Honors

- Radziemski Fellowship — June 2018
  College of Arts and Sciences, Washington State University

Teaching and Mentoring Experience

Lecturer
Washington State University — Fall 2022

- Taught "Physics 150: Physics and Your World".

Graduate Student Instructor — Spring 2018, 2022

- Instructor for "Physics 150".

Physics Teaching Assistant (TA) — Aug 2014 - Dec 2017

- Lab instructor for introduction to physics (Physics 102, 201, 202).

Training and Development

- Attended workshop on "Quantum Turbulence: Cold Atoms, Heavy Ions, and Neutron Stars" — March 2019
  Institute of Nuclear Theory
  University of Washington, Seattle