**APCTP-IACS-SNBNCBS Workshop on Computational Methods for Emergent Quantum Matter: From Theoretical Concepts to Experimental Realization**

**Venue: SNBNCBS & IACS, Kolkata**
**November 17-25, 2022**

**Abstracts for tutorial lectures**

**Workshop Part I : First Principles Method**

### TL 01: Density Functional Theory
Manoj Kumar Harbola
Indian Institute of Technology, Kanpur

Fundamentals of density-functional theory - I
Fundamentals of density-functional theory - II

In these lectures we will discuss basics of density-functional theory with emphasis on exact results. These exact results form the basis for development of new functionals and in analysing and understanding the results obtained by density-functional based calculations.

### TL 02: Density Functional Theory: Status, Achievements, Challenges
Prasanjit Samal
National Institute of Science Education and Research, Bhubneswar

Topic I: Generalized Gradient Expansion (GGA) [Day-1]
Topic II: Meta-Generalized Gradient Expansion (meta-GGA) [Day-2]
Topic III: Hybrid density Approximation [Day-3]
Topic IV: Implementation procedures in codes [Day-4]

Day-3 & Day-4 lectures can be merged if the time limit is short.

### TL 03: GW-BSE Method (TBA)
Manish Jain
Indian Institute of Science, Bangalore

### TL 04: Wannierization and Identification of Topological Phases
Jaejun Yu
Seoul National University, South Korea

Lecture I: Topological ideas in Condensed Matter Systems
   0. Geometric phases in physics
   1. Berry phase and Bloch state:
   2. Berry phase, Berry curvature, and topological invariants
Lecture II: Practical calculations of topological invariants and related properties
   0. Parametric Hamiltonians
   1. Topological bands, Wilson loops, and Wannier functions
   2. Computing Berry connection in Discretized BZs

3. Examples

**References**

- D. Vanderbilt, Berry Phases in Electronic Structure Theory: Electric Polarization, Orbital Magnetization and Topological Insulators. Cambridge: Cambridge University Press, (2018). – doi:10.1017/9781316662205
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- S. Baidya, S. Kang, C.H. Kim, and Jaejun Yu, Chern insulator with a nearly flat band in the metal-organic-framework-based Kagome lattice, Sci Rep 9, 13807 (2019). – https://doi.org/10.1038/

**TL 05: Magnonic analogs of topological insulators in 2 and 3 dimensions**

Hosho Katsura

University of Tokyo, Japan

Magnons (spin waves) are collective excitations in magnets responsible for their magnetic and thermal properties. Recently, there has been a growing interest in studying magnetic systems with nontrivial magnon band topology. However, examples discussed so far have been mostly limited to systems which can be thought of as a magnonic analog of integer quantum Hall systems. In this talk, I will talk about a class of magnonic systems that are the natural counterparts of time-reversal symmetric topological insulators in two and three dimensions [1,2]. The feature of these systems is that each pair of bands related by pseudo-time-reversal symmetry carries a Z2 topological invariant. I will demonstrate that the Z2 invariant so defined characterizes the presence/absence of helical edge/surface modes. If time permits, I will touch on magnonic analogs of topological crystalline insulators [3].

[1] H. Kondo, Y. Akagi, and H. Katsura, Phys. Rev. B 99, 041110(R) (2019).
[2] H. Kondo, Y. Akagi, and H. Katsura, Phys. Rev. B 100, 144401 (2019).
[3] H. Kondo and Y. Akagi, Phys. Rev. Lett. 127, 177201 (2021).

**TL 06: Configuration interaction approach and its applications
to the optical absorption spectra of finite systems**
Alok Shukla
Indian Institute of Technology, Bombay

Treatment of electron correlation effects is one of the most challenging problems in quantum many-electron physics. Several approaches such as many-body perturbation theory, Monte-Carlo approach, coupled-cluster theory, Green's function method, configuration interaction approach etc. are available to treat electron correlation effects from first principles. In this talk we will discuss the configuration interaction (CI) method for computing electron correlation effects on the ground and excited states of finite systems, and discuss its pros and cons. Furthermore, optical absorption spectra of several finite systems such as clusters, pi-conjugated moleculess, and graphene quantum dots computed using the CI method will be presented and discussed.

## Workshop Part II: Model Hamiltonian based approaches

**TL 07: Introduction to Density Matrix Renormalization Group (DMRG) method.**
Suryanarayana Ramasesha
Indian Institute of Science, Bengaluru 560012

Lecture 1: Introduction to Numerical Many-Body Techniques

In this talk, we begin with basic approximations for electronic structure of molecules and solids, namely Born-Oppenheimer approximation and independent particle approximation. We will introduce methods which go beyond the independent particle approximation. These include configuration interaction methods, coupled cluster techniques. We then introduce model Hamiltonians and methods for solving these by using exact diagonalization and Monte Carlo methods. Limitations of these methods will be touched upon.

Lecture 2: Introduction to DMRG method

This talk will begin with early attempts to develop RG methods for interacting Hamiltonians. We will then introduce the infinite DMRG method and its implementation. The symmetrized DMRG method for desired excited states will be introduced. It will be followed by an introduction to finite DMRG method. We will discuss methods for computing matrix elements. The connection between the DMRG method and the Matrix Product States method. Briefly, MPS method for 2-d lattices, namely PEPS will be introduced and method for obtaining the ground state will also be discussed.

Lecture 3: Dynamical Properties from DMRG method

In this lecture I will discuss methods of computing frequency dependent response functions. This will be followed by introduction to time dependent DMRG. In the first part, Lanczos technique for dynamic response functions will be introduced. This will be followed by an introduction to the

Correction Vector method. Under the time dependent DMRG method, I will discuss the need for adapting space and discuss different algorithm for implementation of tDMRG will be discussed.

### TL 08: Exact diagonalization for quantum spin systems
Tokuro Shimokawa
Okinawa Institute of Science and Technology, Japan

The goal of this tutorial is to understand the principles of the three Lanczos-based methods, Lanczos, Finite-Temperature Lanczos, and continued fraction methods. These methods are important and fundamental to investigate the ground-state and finite-temperature physics, and spin dynamics in quantum frustrated magnets from finite-size systems. We here focus on an S=1/2 XXZ spin model for simplicity. We will also learn how to make S=1/2 ED codes with bit representations and bitwise operations, which are efficient for fast ED codes, and will learn the simplest block diagonalization technique under conserved magnetization via Python ED sample codes [https://github.com/tshimokaw/].

**Literatures:**

"Computational Studies of Quantum Spin Systems" by Anders W. Sandvik, arXiv:1101.3281/AIP Conf. Proc. **1297**, 135 (2010).

"Ground State and Finite Temperature Lanczos methods" by P. Prelovšek and J. Bonča, arXiv:1111.5931/Strongly Correlated Systems. Springer Series in Solid-State Sciences, **176** Springer (2013).

### TL 09: Modern mean field theory (TBA)
Arun Paramekanti
University of Toronto, Canada

### TL 10: Tensor network approach to two-dimensional frustrated spin systems
Tsuyoshi Okubo
University of Tokyo, Japan

In this tutorial, I will introduce the tensor network method for calculating the ground state of quantum lattice models. Specifically, we focus on infinite tensor product states (iTPS), also known as infinite projected entanglement pair states (iPEPS), for infinite two-dimensional systems. We discuss when this method works efficiently, fundamental numerical algorithms for iTPS, and an extension of iTPS for finite temperature properties.

In the Hands-on tutorial, I will introduce an open-source software, TeNeS, for the ground state calculation based on iTPS.

References:

[1]   R. Orús, A practical introduction to tensor networks: Matrix product states and projected entangled pair states, Ann. Phys. (N. Y.), 349 117 (2014).

[2] Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Kato, and N. Kawashima, TeNeS: Tensor network solver for quantum lattice systems, Comput. Phys. Commun. 279, 108437 (2022).

[3] The web page of TeNeS: https://www.pasums.issp.u-tokyo.ac.jp/tenes/en