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

Venue: SNBNCBS & IACS, Kolkata
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Abstracts for perspective talks
Workshop Part I : First Principles Method

PT 01: DFT and Beyond the Materials Design and Discovery

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PT 02: Probing Excited States in Materials: Benchmarking Hybrid DFT vs GW vs BSE vs model BSE

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Oxides and perovskites have always attracted considerable attention as promising materials having wide applications in opto-electronics. However, to date, several key electronic properties such as optical properties, effective mass, exciton binding energy and radiative exciton lifetime are largely unknown. Here, we employ an integrated approach with several state-of-the-art first-principles based methodologies viz. hybrid-DFT combined with spin–orbit coupling, many-body perturbation theory (GW/BSE), model-BSE (mBSE), Wannier–Mott and density functional perturbation theory to address these properties with sufficient accuracy [1-5]. However, for a reasonably large supercell, direct estimation of excited state properties at the level of BSE is rather demanding and sometimes impossible with a sufficiently converged k-mesh and vacant orbitals. Therefore, by taking a prototypical model system, we present how the mBSE approach is carried out to circumvent the computational cost of performing direct BSE@G_0W_0@HSE06 without compromising the accuracy [6].

References:
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[2] P. Basera, M. Kumar, S. Saini, SB Phys. Rev. B 101, 054108 (2020)
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[5] M. Kumar, A. Singh, D. Gill, SB J. Phys. Chem. Lett. 12, 5301 (2021)
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PT 03: Using wannier functions to get insights into the electronic structure

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PT 04: Basic considerations of electronic and magnetic structures of transition metal compounds

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PT 05: From Materials to Models

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In this talk, we will focus on materials modelling methods to allow combining compound-specific and many-body aspects, by adding chemical reality to physically intuitive models. We will start with discussion of short-coming of ab-initio DFT approaches in description of strongly correlated electron systems, followed by extraction of DFT essentials in derivation of material-specific many-body model Hamiltonians to be solved by a variety of many-body techniques. Examples will be drawn from High Tc cuprates, low-dimensional spin systems, magnetic double perovskite compounds.

PT 06: Higher-order topology in quantum spin models

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The concept of free fermion topology has been generalized to d-dimensional phases that exhibit (d − n)-dimensional boundary modes, such as zero-dimensional (0D) corner excitations. In this talk, I will first briefly introduce the notion of Higher-order topological (HOT) phases. Following the introduction, I will talk about extending HOT phases to spin systems and discuss the theoretical prediction of HOT-triplons in quantum paramagnets formed by interacting spin dimers.

Workshop Part II : Model Hamiltonian based approaches

PT 07: Why has it been so difficult to arrive at a consistent theory of superconductivity in the high Tc cuprates?

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More than three decades after the discovery of superconductivity in the cuprates, the nature of the “normal” state and the mechanism of superconductivity remain mysterious. The overall confusion has actually increased recently, stemming from the convincing demonstration of nonsuperconducting ground state within the optimally doped purely two-dimensional (2D) Hubbard Hamiltonian [1]. The numerical results of reference [1] have pointed out the deficiencies of the many different approximate theories that do find cuprate superconductivity based on the 2D Hubbard model. Whether or not superconductivity will be found upon inclusion of second neighbor hopping or by going over to the multiband Hubbard model is still being debated.

In this talk I will present the viewpoint that theoretical efforts to understand cuprate superconductivity have missed the key concept of valence transition, that has been discussed previously in the context of materials as diverse as heavy fermions [2] and organic donor-acceptor charge-transfer solids [3]. I will point out that this concept allows us to construct a “global approach” to the slew of diverse “negative charge-transfer gap” materials [4]. Following this I will present our recent work on the cuprate ladder superconductor Sr2−xCaxCu24O41 [5,6], which provides strong support to the valence transition approach to pseudogap, charge-order and superconductivity in the layered cuprates [7]. Time permitting, I will discuss the application of the theory to Sr2RuO4 [8].

References:
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PT 08: Protecting quantum criticality

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According to the standard correspondence between a quantum many-body system and a classical statistical system, a quantum critical point corresponds to a critical point which is realized only by fine-tuning of parameters. However, there are quantum critical phases which are apparently stable without any fine tuning. I will review some of the mechanisms which protect quantum criticality, including Lieb-Schultz-Mattis type theorems and recently proposed gapless Symmetry-Protected Topological phases.

PT 09: Detection of Majorana zero mode in Kitaev’s honeycomb spin liqiud

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Kitaev's spin liquid is drawing considerable attention as a realistic stage of long-sought quantum spin liquid (QSL) phase. Among its fascinating properties, the field-induced chiral spin liquid (CSL) state deserves special attention, where the half-integer quantization of thermal Hall conductivity is theoretically predicted, and is experimentally reported for one of the candidate materials, alpha-RuCl3 [1].
The appearance of Majorana zero mode (MZM) is another remarkable phenomenon expected in the CSL phase. A fractional excitation called vison accompanies MZM and behaves as a non-Abelian Ising anyon. Experimental detection of this novel quasiparticle opens an avenue to topological quantum informatics in a material.

In this talk, we first introduce the dynamics of Kitaev's model with an emphasis on the exact analytical expression of finite-temperature dynamical correlation function of this model [2,3]. With the knowledge of the dynamical response, we discuss recent theoretical proposals to detect MZM in Kitaev's QSL through the spectroscopic experiments such as the scanning tunneling microscopy [4]. We also introduce recent attempts to control the position of visons with external probes [5].

References:
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PT 10: Flat bands and related topics

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Recently, flat-band systems have attracted much attention. Since the kinetic energy is completely quenched in such systems, the effect of interactions is essentially non-perturbative. Interestingly, they often allow for an exact treatment of many-body problems. In this talk, I will first review various methods for constructing tight-binding models with exactly flat bands. I will then introduce interaction terms and review rigorous results concerning ferromagnetism in the Hubbard-type models. If time permits, I will also discuss some other topics.

PT 11: Emergent behavior at low and high energies in some frustrated magnets

Arnab Sen
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PT 12: Matrix product states as an efficient ansatz for strongly correlated systems

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Polyaromatic hydrocarbons, polyenes, metal clusters are all strongly correlated systems, difficult to solve with traditional quantum chemistry methods. Earlier studies have already noticed that use of complete valence active space is imperative to the understanding of its qualitative and quantitative properties. Since complete active space based methods cannot be applied to such large active spaces, we have used density matrix renormalization group (DMRG) based approaches. 1,2 This is an incredibly efficient approach for 1-D systems, but are plagued with difficulties for 2-D systems. We, therefore, develop artificial neural network based configuration interaction approaches 3 and its extension to solve matrix product state ansatz wavefunctions.

References:

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