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Abstract Details

Kondo effect in open quantum systems

N S Vidyadhiraja, JNCASR, Bangalore

The Kondo effect is a standard paradigm in quantum many-body systems, wherein discrete degrees of freedom hybridize with a continuum, and due to strong local interactions, a new low energy scale associated with dynamical screening effects emerges. However, the fate of Kondo effect in open quantum systems is not yet known. We use the framework of non-Hermitian quantum mechanics to investigate the interplay of strong interactions, spin-orbit coupling, and PT-symmetry in an open quantum dot-lead system. Several interesting results regarding exceptional points in the non-interacting case will be discussed. Using the slave-boson approach, we show that spin-orbit coupling and strong interactions act co-operatively, and induce a line of Kondo destruction type quantum critical points. Some open questions regarding the relation of quantum criticality and violation of PT-symmetry will be outlined.

Non-equilibrium dynamics of Solvent around Laser-Heated Janus Colloids

Sutapa Roy, IIT Gandhinagar

Laser illuminating a Janus colloid which is suspended in a near-critical solvent leads to the formation of the concentration gradient and coarsening patterns around the colloid, which leads to its phoretic motion. Using analytical theory and numerical simulations, we investigate this non-equilibrium phenomenon under the influence of a time-dependent temperature gradient. Our predictions are also confirmed by experiments with Gold-capped Janus particles immersed in PnP-water liquid mixture. Time-dependent properties of the coarsening patterns for various surface adsorption properties of the Janus colloid are analyzed. We also present results for structure formation around colloidal particles kept confined in thin films with confining surfaces preferring one species of the binary liquid mixture over the other. Results will also be presented for effective forces between multiple colloidal particles.

DIFFUSION AND SINTERING OF ULTRASMALL NANOPARTICLES: MECHANISMS & SCALING RELATIONS

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Small nanoparticles supported on substrates are of technological interest because they can be excellent catalysts for many industrially and environmentally important reactions. They can also possess interesting physical properties, e.g., small particles of some elements can be nanomagnets, even if the corresponding bulk material is non-magnetic. Properties of interest, such as chemical reactivity and magnetic moments, are highly size-sensitive -- typically, the catalytic activity of metal nanoparticles increases sharply as the size is decreased. However, nanoparticles are intrinsically unstable with respect to sintering: it is always energetically favorable for two or more nanoparticles to coalesce to form a larger-sized particle. This process is one of the important causes of nanocatalyst degradation. It is therefore of interest to study the processes by which nanoparticles diffuse on substrates, and fuse together.

I will present work in our group on the diffusion and sintering of ultrasmall small noble metal particles on a MgO support. We find that these clusters diffuse by unexpectedly complex motions that do not correspond to simple translations. The diffusion mechanism depends upon both the atomic species and the number of atoms in the nanoparticle. We find unexpected scaling relations between diffusion barriers and other quantities (such as the melting temperature of the bulk metal), we will discuss the origin and implications of such scaling relations.

This work was done jointly with my former student Nisha Mammen.

Theory of a benzene transistor: symmetry, strong correlations and quantum interference

Sudeshna Sen, IIT(ISM) Dhanbad, Jharkhand

Single molecule transistors offer a fascinatingly diverse range of physics beyond the capabilities of Si transistors. Their ultrasmall size, chemical complexity, and electronic interactions constitute a unique playground for exploring the fundamental physics of correlations on the nanoscale, and their transport signatures. Understanding these systems is an essential prerequisite for possible advanced technological applications utilizing their quantum characteristics. In this talk I examine the interplay of symmetry and Kondo effect in a benzene single electron transistor using a combination of numerical renormalization group and generalised Schrieffer Wolff transformation. Depending on the connectivity of the leads and gate voltages, we uncover spin-1/2 and spin-1 Kondo effects, a quantum phase transition to a state with robust molecular magnetism, and destructive quantum interference at an emergent SU(4) symmetry point. The interplay between emergent many-body effects and molecular symmetry is discussed in the context of quantum-boosted device functionality.

Binary- and Ternary-fluid Turbulence: An Introduction

Rahul Pandit, IISc, Bagalore

I will begin with examples of binary- and ternary-fluid flows and of turbulence in such flows. I will then introduce the Cahn-Hilliard-Navier-Stokes (CHNS) equations for such binary and

ternary fluids. I will give some illustrative results from (a) our direct numerical simulations of such flows and (b) a regularity criterion for the solutions of the three-dimensional CHNS equations.

This talk is based on studies that I have carried out with: Nadia Bihari Padhan, Department of Physics, IISc, Bangalore; Nairita Pal, Los Alamos National Laboratory, USA; Prasad Perlekar, TCIS TIFR, Hyderabad; John D. Gibbon, Department of Mathematics, Imperial College, London; Anupam Gupta, IIT, Hyderabad. I would like to acknowledge support from CSIR, SERB, NSM, UGC, and SERC (IISc).

Sufficient Statistic in Quantum Theory

K B Sinha, JNCASR, Bangalore

In many fundamental questions in Statistical Methodology, the concept of a "sufficient statistic" plays a central role. Such concepts or related ideas had been used in Quantum Theory in the study of Symmetries in the Physical systems, with the goal of a systematic reduction of the problem. These relationships are studied thru a few examples.

Flat-band-induced non-Fermi-liquid behavior of multicomponent fermions

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We investigate multicomponent fermions in a flat band and predict experimental signatures of non-Fermi-liquid behavior. We use dynamical mean-field theory to obtain the density, double occupancy and entropy in a Lieb lattice for $N = 2$ and $N = 4$ components. We derive a mean-field scaling relation between the results for different values of N , and study its breakdown due to beyond mean-field effects. The predicted signatures occur at temperatures above the Néel temperature and persists even in the presence of a trapping potential, thus they are observable in ultracold gas experiments.

Reference:

Pramod Kumar, Sebastiano Peotta, Yosuke Takasu, Yoshiro Takahashi, and Päivi Törmä, Flat-band-induced non-Fermi-liquid behavior of multicomponent fermions, **Phys. Rev. A** 103, L031301 (Letter)

Novel Nanocatalysts from Ligand-Stabilized Metal Nanoclusters

Nisha Mammen, Univ of Jyväskylä

The hallmarks of a good nanocatalyst are high stability against degradation, high reactivity (low energy barriers) and high selectivity towards a desired product. Ligand-stabilized, atomically precise nanoclusters are a fundamentally new class of nanomaterials that could potentially offer these desired characteristics. However, there is still much to be understood regarding whether the ligands need to be on or off for the catalyst to be active, role of the ligands during catalysis if they are still on and catalytic mechanisms involved. Gaining information about these issues helps pave the path forward towards the rational design of such catalysts.

In this talk, I will present results from our density functional theory calculations and molecular dynamics (MD) simulations with DFT-based forces, performed to investigate in detail the atomic dynamics in the ligand layer of two *meta*-mercaptobenzoic acid (*m*-MBA) stabilized gold clusters, viz., Au₆₈(*m*-MBA)₃₂ and Au₁₄₄(*m*-MBA)₄₀. These clusters are unique as they exhibit three new interactions not observed in clusters of similar sizes. They have weak ligand-ligand interactions O=C-OH...O=C-OH, as well as two weak ligand-metal interactions, viz., O=C-OH...Au and Ph(Π)...Au.¹ Due to the highly dynamic nature of these weak interactions, they are being continuously formed and broken. Based on this, we had hypothesized that these weak ligand-gold interactions could open a new dimension in the discussion of the role of ligands when these clusters are used as catalysts. In our most recent work, we reported that these clusters can indeed be stable, selective, mild temperature catalysts for the partial selective hydrogenation of acrolein to an unsaturated alcohol. The weak ligand-gold interactions, in particular the Ph...Au interaction, are easily sacrificed to expose highly mobile, low coordinated Au atoms on the surface of the cluster that act as active sites for the catalytic reaction. The opening of these interactions to trap reactant molecules at Au sites is similar to the mechanism observed in a *Venus-flytrap* where the flowers of the plant exhibit motion to trap their prey.²

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Genomics signatures of host-parasite coevolution

Sona John, Technical University of Munich, Germany

Host-parasite coevolution is a well-known example of inter species interaction which has evolutionary consequences in both partners. Detecting the genomic regions under coevolution is of great interest in disease control and drug design. Different genomic regions are expected to contribute differently to the coevolution based on its functionality. Some regions are expected to impact the process substantially, those we call it as the major genes. Regions that have milder effects are called minor genes. Also, some regions that do not influence the coevolution process are called neutral genes. This study aims to identify the genomic signatures of coevolution in each of these regions.

Post Translational Modifications Induced Structural Reorganization in Tau Protein

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Microtubule associated protein Tau (MAPT) is a phospho-protein within neurons of the brain. Aggregation of tau is the leading cause of tauopathies such as Alzheimer's disease. Tau undergoes several post-translational modifications of which phosphorylation and O-GlcNAcylation are key chemical modifications. Tau aggregates into paired helical filaments (PHF) and neurofibrillary tangles upon hyperphosphorylation whereas O-GlcNAcylation stabilizes the soluble form of Tau. How specific phosphorylation and/or O-GlcNAcylation events influence Tau conformations remains largely unknown due to the disordered nature of Tau. We have investigated the phosphorylation and O-GlcNAcylation induced conformational effects on the proline-rich domain (P2) and the R3-R4 repeat domains of human Tau protein. PTMs were introduced at experimentally verified phosphorylation and O-GlcNAcylation sites. Our studies suggest the opposing structural effects of both PTMs and the importance of salt-bridges in governing the conformational preferences upon phosphorylation, highlighting the role of proximal Arginine and Lysine upon hyper-phosphorylation. The structural effects upon PTM were found to be prominent for phosphorylation when compared to O-GlcNAcylation. One of the key observations from our study was the conformational transition to a more opened "H-conformation" upon phosphorylation when compared to the compact "C-conformation" observed

in native Tau PHF.¹⁻³ The study sheds light on the structural implication of PTMs paving the way for further investigations.

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2D materials in the spot"light": the emergence of advanced optical properties

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Moore's law that dictated the miniaturization in silicon electronics since 1965, has begun to fail in recent years indicating approaching limit in size reduction of conventional silicon-based electronics. To overcome this obstacle, scientific efforts have focused on potential silicon replacement - "two-dimensional" (2D) materials, that exhibit exotic properties due to quantum confinement effects, leading to enhanced response to external fields. Using first-principles theory, I will discuss the emergence of exceptional optical properties in 2D materials. First, building on simple electronic models, I will show how dimensionality affects the maximum achievable reflectance and absorbance in 2D materials[1]. Amazingly, dimensionality reduction strikingly amplifies properties of some materials for use as ultrathin reflectors and absorbers in various frequency ranges of the electromagnetic spectrum, that surpass the performance of conventional thin films. Furthermore, by tuning the free carrier density in 2D metals, I will show that light-matter interaction induces visible frequency plasmons that allow nanoplasmonic devices to squeeze information with 100 times higher resolution[2]. This work explores the fundamental physics behind advanced functionalities in 2D materials, that find promising applications in technological areas of nanoplasmonics and optoelectronics.

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Estimation of the equilibrium free energy for glasses using the Jarzynski equality

Vinutha H A, Georgetown University, United States

The free energy of glasses cannot be estimated using thermodynamic integration as glasses are intrinsically not in equilibrium. We present numerical simulations showing that, in contrast, plausible free-energy estimates of a Kob–Andersen glass can be obtained using the Jarzynski relation. Using the Jarzynski relation, we also compute the chemical potential difference of the two components of this system and find that, in the glassy regime, the Jarzynski estimate matches well with the extrapolated value of the supercooled liquid. Our findings are of broader interest as they show that the Jarzynski method can be used under conditions where the thermodynamic integration approach, which is normally more accurate, breaks down completely. Systems where such an approach might be useful are gels and jammed glassy structures formed by compression.

Multi-Scale Modelling and Theory of Structural Phase Transitions

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Properties of a material are fundamentally determined by its structure, and hence sharp changes in its structure marking a structural phase transition have remarkable impact on its behavior. Symmetry breaking at such a phase transition typically is a cause for emergence of technologically important functional properties. For example, use of a ferroelectric in sensors, speakers or in memories is possible due to piezoelectricity and switchable dipole moments it exhibits as a consequence of broken inversion symmetry. For development of advanced functional materials, it is thus highly desirable to have *material-specific* theory of structural phase transitions, which often involve many symmetry breaking structural fields and processes that occur at many time and length scales.

We first present an account of how the principles of coarse-graining in time and spatial domains

can be used to develop realistic, material-specific models from first-principles quantum theoretical description of a material. Starting with accurate picture of chemical bonding in terms of electronic motion in a material, these facilitate bridging of descriptions of a materials at multiple scales and capturing its temperature and pressure dependent structural phase transitions through statistical mechanical analysis with Monte Carlo (MC) and Molecular Dynamics (MD) simulations.

We illustrate this scheme with application to ferroelectric transitions in perovskite oxides, Neel transition in hexagonal manganites, martensitic phase transformation in shape memory alloys and electronic structural transitions in excitonic insulators.

Flow and flow cessation properties of soft dense disordered materials

Vishwas Vasisht, IIT Palakkad

Soft disordered materials form a major part of our daily life including colloidal suspensions like paste, foam, paint, bitumen, wet cement etc., At high densities, these suspensions behave like an athermal disordered solid. Upon shear deformation, the material yield and eventually flow like a viscoelastic fluid. The yielding behavior is quite rich, and has gained a lot of attention in the recent years. During the yielding, the material often display an overshoot in stress before decaying towards a steady state stress. The approach to the steady state can be accompanied by heterogeneous flow properties termed as shear bands. These heterogeneity are transient in nature, but the time to reach a uniform flow doesn't trivially scale as inverse shear rate. With the decrease in the background viscosity (inertial systems) the shear bands can persist for ever and are termed as permanent bands. Upon cessation of the flow (stopping the shear deformation), the stress in these materials do not decay to zero even after a long time. The material retains certain residual value and this residual stress depends material's microscopic properties during the steady state flow. In this talk, I would try to accommodate all these fascinating features of the soft dense disordered materials.

Mpemba Effect: Surprizing, yet common?

Subir K. Das, JNCASR, Bangalore

Should a hotter body of water freeze quicker than a colder one when quenched to a common subzero temperature? This surprizing question is closely related to the domain of nonequilibrium statistical physics. An answer in affirmative is counter-intuitive and is now known as the Mpemba effect (ME). Despite having its mention in the writings of Aristotle, Descartes and the likes, there still exists controversy on the very existence of the effect. On the other hand, there are efforts to discover ME-like effect by asking the general question: Should a hotter body of a material equilibrate faster than a colder one when quenched to the same lower temperature? Evidences have been reported in a few systems other than water. However, a class of studies provide an impression that frustration or metastability is essential for the exhibition of the effect.

In this talk I will discuss results showing evidence of the effect even during para-to-ferromagnetic transition in the q-state Potts model, despite the model containing no in-built frustration. The controversial case of water will also be discussed.

Crystal nucleation and liquid-liquid transition in supercooled silicon

Srikanth Sastry, JNCASR, Bangalore

The possibility of a liquid-liquid transition in several network forming liquids including water, silica and silicon have been investigated intensely over several years. While many computer simulations showed evidence of such a transition in several substances, these putative transitions in most cases occur in the supercooled liquid regime, and therefore the kinetics of crystallisation in principle influences the ability to observe such a transition. It has even been argued that the evidence claimed for a liquid-liquid transition arises from misinterpretation of slow crystallisation. Robust evidence for a liquid-liquid transition has been generated in the case of several computer models of water by constructing a free energy surface that displays distinct minima for the different liquid phases, as well as a clear barrier to crystal nucleation. Similar results have not been available in the case of supercooled silicon. Recent results regarding kinetics and thermodynamics relevant to the liquid-liquid transition phenomenology, obtained through analysis of computer simulations of a classical model of silicon, will be presented.

Slow quench dynamics in classical systems

Kavita Jain, JNCASR, Bangalore

The phase ordering dynamics of a system following an instantaneous quench have been well studied but such dynamics have been relatively less explored when the quench occurs at a finite rate. I will describe our analytical and numerical results on a kinetic Ising model and a zero range process when the system is annealed slowly to the critical point. Starting from the time-evolution equations, we derive the Kibble-Zurek scaling laws for the defect density at the critical point and elucidate the role of critical coarsening in the approach to the critical point.

Multiscale lattice dynamics and emergent phenomena: Flexibility and Boson peaks of crystalline materials

Meha Bhogra, Shiv Nadar University

In this talk, I will highlight two interesting phenomena emerging from multiscale lattice dynamics and strain-phonon coupling -- flexibility and Boson peaks, using metal-organic

frameworks (MOFs) as the model crystalline materials. Flexibility of a solid is associated with its ability to accommodate reversible changes in shape and size. While it is widely used to describe physical and biological processes, its quantitative measure and fundamental origin is presently lacking. Drawing on the phenomenology of flow in liquids, we introduced intrinsic flexibility of crystalline materials as the fractional release of elastic strain-energy through symmetry-preserving internal structural rearrangements. Using first-principles theoretical analysis, we uncovered unexpectedly comparable contributions from soft as well as hard vibrations, that couple strongly to strain fields, to flexibility of crystals. In the second half of my talk, I will show that Boson peak (BP), a characteristic of amorphous (disordered) and glassy systems, can appear in ordered crystalline materials, thus invalidating the applicability of simplistic Debye model to complex crystals. With the emergence of BP from composite modes in one MOF, and shear modes in the other, we elucidated that the lattice vibrations that constitute the BP are not quite universal, and strongly depend upon the underlying topology and chemical interactions in the crystal.

First-Principles Modelling of Optoelectronics and Charge-Transport in Functional Molecules and Materials

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Development of functional molecules and materials can greatly benefit from an in-depth understanding of their complex structure-property relationships at the microscopic level. This is sometimes very difficult to achieve using sophisticated experimental techniques and therefore, in practice becomes a challenging task. To this end, first-principles based simulations not only complement experimental observations through unravelling microscopic details, but also can provide predictions for novel materials. However, such predictions are often highly dependent on the methodological choice, for an example density functional used in density functional theory (DFT) and time-dependent DFT.

Reliable description and quantitative predictions can be obtained with carefully designed DFT functionals that maintain a delicate balance between the amount exchange and correlation, and also simultaneously satisfy certain necessary constraints. Non-empirically and optimally tuned system-dependent range-separated hybrid that includes an admixture of Fock and DFT exchange in the short-range and full Fock-exchange in the long-range has been proven to yield physically meaningful orbitals and accurate excited-state properties in a range of molecular systems.¹ In this talk, I shall present and discuss some of our recent results on both optical and charge-transfer properties in a few π -conjugated molecules from optimally tuned range-separated hybrid and

screened range-separated hybrid.²⁻⁴ Importantly, an appropriate choice of DFT functional combined with suitable theoretical protocols can indeed produce reliable and accurate description of such molecular properties in vacuum and also in the condensed-phase environment.

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Multiple proton transfers in Molecular Crystals: Role of nuclear quantum effects

Prasenjit Ghosh, IISER Pune

Multiple hydrogen/proton transfer (intra- or intermolecular) (MPT), both in the ground and excited state, is important in several biological and chemical processes. One of the open questions in this area is whether MPT involves a concerted process or occurs in a stepwise manner. Additionally, H atoms being the lightest element in the periodic table, it would also be natural to ask how NQE affects MPT processes: do these effects make MPT less or more concerted? To answer these questions, there have been recent computational and experimental studies that have looked into double proton transfer (DPT) in single molecules (intra molecular) in gas phase or on transition metal substrates. However, there are very few available reports of intermolecular DPT and those too, are in complex biological systems where it is very difficult to separate out how different factors like molecular interactions and the environment affect DPT. In contrast, studying DPT in H-bonded molecular crystals, where there is long range order, will help in a better understanding of how the different factors affect DPT. However, to the best of our knowledge, there are hardly any studies involving DPT in molecular crystals.

In order to shed some light on the above mentioned issues, in this work, using path integral molecular dynamics simulations, we have investigated DPT in a H-bonded molecular crystal, terephthalic acid (TPA). A TPA molecule consists of two –COOH groups on the opposite sides of a benzene ring. In TPA crystals, molecules bind together through H bonds between these -COOH groups forming long chains. As a result, between a pair of molecules there are two H-bonds, resulting in the possibility of occurrence of a double proton transfer. In addition to this double proton transfer, these crystals are known to undergo order-disorder transitions at around 70 K. In this talk, I would provide answers to some of the following questions:

- (a) What is the nature of the double proton transfer? Is it stepwise or concerted?

- (b) Are there any correlations between DPT occurring at two different H-bond sites (both intralayer and interlayer)?
- (c) How do molecule-molecule interactions and the crystal-field affect the double proton transfer?
- (d) How are the proton transfer and their correlations (if any) modulated by nuclear quantum effects?
- (e) Since the proton/H is significantly delocalized due to NQE, is there any coupling between the proton and electronic degrees of freedom?

Quantum Modeling of Molecules and Materials for Various Applications

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We have been developing various quantum methods to describe charge transfer, generalized transport, optical and magnetic phenomena which occur in various miniaturized devices. I shall discuss a few projects that my lab members are working currently: from light harvesting, development of cathode materials, perovskite solar cells, inducing hot-carrier cooling in various hetero-structure(s), designing thermoelectric materials to frustrated Lewis pair based catalysis and heterogeneous catalysis [1-10]. We also had developed both voltage-constraint and current-constraint approach to understand current-voltage characteristics in molecules and quantum dots in the strong coupling regime, and Master Equation (Kinetic Equation) approach in the weak coupling regime. I shall discuss two recent works on quantum dots in weak coupling regime using quantum many body theory coupled with Kinetic Equation formalism [11-12].

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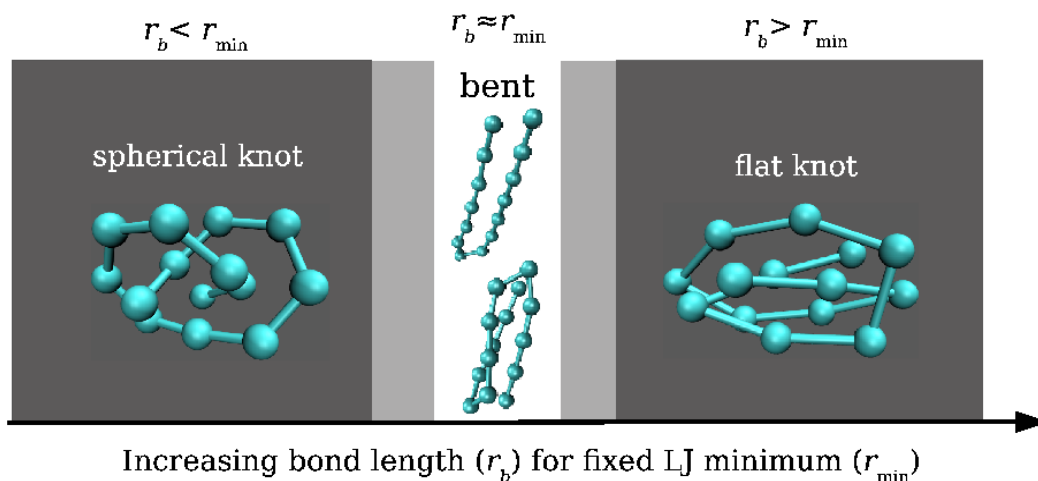
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Title: Knots are Generic Stable Phases in Semiflexible Polymers

Authors: Suman Majumder*, Martin Marenz, Subhajit Paul, and Wolfhard Janke

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Abstract: While investigations of knots in polymers have lured scientists for decades, the existence of phases characterized by a stable knot of specific type has attracted attention only recently. In this work, we treat two popular models that encompass the complete spectrum of real polymers (flexible to stiff) via extensive replica exchange Monte Carlo simulations, and show that the existence of stable knots in the phase diagram depends only on the ratio r_b/r_{\min} , where r_b is the equilibrium bond length and r_{\min} is the distance for the strongest nonbonded contacts in an attractive Lennard-Jones (LJ) potential. Our results provide evidence that irrespective of the model, bead-stick or bead-spring, if the ratio r_b/r_{\min} is outside a small window around unity then one always encounters for semiflexible polymers stable knotted phases at low temperatures.



Reference: S. Majumder, M. Marenz, S. Paul, and W. Janke, *Macromolecules* **54**, 5321-5334 (2021).

Exclusion Process with Dynein inspired dynamics

Priyanka, University of Illinois, Urbana-Champaign, USA

Motivated by the sidewise motions of dynein motors shown in experiments, I will talk about a variant of the exclusion process to model the multistep dynamics of dyneins on a cylinder with open ends. Due to the varied step sizes of the particles in a quasi-two-dimensional topology, there is an emergence of a novel phase diagram depending on the various load conditions. Under high-load conditions, our numerical findings yield results similar to the TASEP model with the presence of all three standard TASEP phases, namely the low-density (LD), high-density (HD), and maximal-current (MC) phases. However, only the LD and HD phase for all chosen influx and outflux rates are observed for medium- to low-load conditions, and the maximal-current phase disappears. Further, I will also talk about a single dynein particle with slower dynamics than a TASEP particle in a crowded environment. Interestingly, the results also confirm experimental observations of the dwell time distribution: The dwell time distribution for dyneins is exponential in less crowded conditions, whereas a double exponential emerges under overcrowded conditions.

Refs: *Riya Nandi and Priyanka, J. Stat. Phys vol.182 (2021)*

Riya Nandi, Uwe C Tauber, and Priyanka, Entropy, vol 23(10) (2021)

Trace formula for pair of contractions

Arup Chattopadhyay, Indian Institute of Technology Guwahati

Krein's trace formula and the associated spectral shift function originated from Lifshits' work on theoretical physics and the mathematical theory of this object was first founded by M.G. Krein. The spectral shift function has become a fundamental object in perturbation theory and it can also be recognized as the scattering phase and the spectral flow in a non- commutative geometry setting. In this talk, first I will talk about Krein's trace formula corresponding to a pair of self-adjoint operators. Next, I will briefly discuss Krein's trace formula for a pair of unitary operators via Cayley transform. Finally, at the end we will discuss trace formula for pair of contractions as an independent mathematical interest, a recent joint work with Kalyan B. Sinha.

