Nonequilibrium tricritical behaviour in the driven XY ferromagnet

Muktish Acharyya
Presidency University

In this talk, I will show the recent Monte Carlo results of studies on XY ferromagnet driven by elliptically polarised magnetic field wave. The discussion will be focused on the nonequilibrium tricritical behaviour and the phase diagrams.

Rough or crumpled: Phases of a generalised Kardar–Parisi–Zhang equation

Abhik Basu
Saha Institute of Nuclear Physics

TBA

: *Separation of inertial active particles in a confined channel*

P S Budara
Indian Institute of Technology Kharagpur

Active particles differ from passive particles in their degree of freedom. Passive particles move randomly due to thermal fluctuations, whereas active particles show self-propelled motion. In this talk, I will discuss the diffusive behavior of interacting, inertial active particles in an asymmetric channel. The particles are subjected to an external oscillatory force along the length of the channel. In the absence of interaction, the mean velocity of the particles shows maximum for moderate mass, i.e., particles of moderate mass have higher velocities than the rest. In the presence of interaction, mean velocity exhibits an additional peak at lower mass, indicating that particles of lower and moderate mass can be separated simultaneously from the rest. I will present the empirical relations for estimating the optimal mass values as a function of interaction strength, the self-propelled velocity, and the parameters of the oscillatory force. These findings are beneficial for particle separation.

Correlated orientational disorder in crystalline assemblies of hard convex polyhedra

Avisek Das
Indian Association for Cultivation of Sciences

Entropy driven self-assemblies of hard convex polyhedral into simple and complex crystals have been valuable model systems for understanding colloidal crystals and superlattices formed by anisotropic nanoparticles. The nonspherical shapes of the building blocks lead the possibility of crystalline phases with purely orientational disorder. Here, despite maintaining a specific crystal structure, defined in terms of center of geometries of the particles, particles adopt different orientations, with no discernible relationships with the underlying crystal structure. We report computational evidence of a new type of orientational phase in the cubic crystals formed by certain hard convex polyhedral. Despite the lack order, particle orientations are not random and exhibit strong correlations. The novel forms of orientational correlations observed in multiple systems seem

to follow a common pattern characterized by certain conserved features. The rotational motions of particles are found to be restricted between a small set of unique orientations with three properties. The number of such absolute orientations is fixed for a shape and does not change between multiple realizations of the system. Irrespective of external pressure, particles are always equally distributed among these special orientations. While doing so, the pairwise orientational differences between the unique orientations are always conserved and are also properties of the shape and nothing else. The result of the correlations is a "discretely mobile" phase at low packing fraction and an orientationally arrested state at high pressures, where each particle is frozen in one of the unique orientations, maintaining the relationships These three conserved quantities are the defining features of the new phase, which is qualitatively different from the known form orientational disorder, namely the plastic crystal phase. In the hard polyhedral systems, the plastic crystals are known to have a continuous mobility, where particles adopt all possible absolute orientations while preserving the positional arrangement of the crystal. The new orientational phase can be termed as a "correlated orientationally disordered" phase because of the presence of both attribute and novel form of specific correlation defined by the conserved quantities. The apparent dichotomy of non-random particle orientations and the notion of disorder across the system can be reconciled by the analyzing orientational nature of the unit cells the crystal is composed of. It turns out that due to presence of the large number of orientationally distinct unit cells, the system could adopt a maximally random composition at the unit cell level, despite conforming to a very limited nature of discrete disorder at the single particle level. With decreasing pressure, the correlated disordered phase transitions into either into a completely random plastic crystal phase, giving rise to a purely orientational solid-sloid transition in the phase diagram or directly into isotropic liquid without the existence of any other solid phase. The origin of orientational correlations appears to stem from a underlying symmetry consideration involving the point group symmetry of the anisotropic particle and the rotational symmetry of the crystal unit cell, which happens to be the one for the cubic system for all occurrences of the correlated disordered phase. It was empirically observed that for every particle in this new phase, the highest order rotational symmetry axis of the particle was always parallel to one of the rotational axis of the crystal unit cell. This finding seems to provide a straightforward justification of the presence of distinct orientations and the number of such special orientations. It appears that the main factor determining the presence of this phase is the mismatch of two kinds of symmetries mentioned before. Shapes with point groups with order much smaller than that of the full octahedral point group of cubic crystals tend to form this phase. A systematic variation of particle shapes further indicated that it the symmetry alone and not any other geometric properties of the shape that is the determinant of the existence of this phase. In summary, our recent results suggest rich phase behaviors of hard polyhedral crystalline systems involving particle orientations and this emergent properties appears to have a fundamental origin rooted in important symmetries of the system. In the context of self-assembly, our findings further emphasize the versatility of entropy as organizing principle and particle shape as design principle in understand phase behavior of soft matter systems.

Josephson oscillations and chaotic dynamics near ultracold atom-dimer resonance

Raka Dasgupta
Calcutta University

We consider a process of trimer formation in a resonantly paired atom-dimer system. It is treated as a two-step process where two bosons first combine to form a dimer, following which an atom collides with this dimer to form a trimer. The Feshnach detuning d1 and d2 corresponding to these two resonances are the crucial adjustable variables in this model. We study the mean-field dynamics of the system. We show that the Josephson oscillation of the collective atomic motion leads to a particle-localization transition. In addition, it is found that in the d1-d2 space, one can find regions over which chaotic behaviour is observed.

Obtaining Insights into the Molecular Mechanisms in Biology using MD Simulations

Shubhra Ghosh Dastidar
Bose Institute

Proteins, being the polymers of α-amino acids, have incredible number of accessible conformations. But for each protein, only a small region of that vast conformational space is relevant for function, which is known as the native state and it is also likely to be the most populated region in the conformational space. Molecular Dynamics (MD) simulation-based sampling methods, focused around ensemble of conformations in the vicinity of the native state have been proven to be useful to provide mechanistic insights into the processes in biology. While the statistical significance of the sampling timescale is important to claim the results to be realistic, in practical sense the timescales of the biological processes are still several fold higher than that the state of art computers can access. Nevertheless, strategic applications of such methods, could be useful to address questions which have much relevance in biology, e.g. obtaining insights into the cell proliferation or even finding suitable inhibitors for a flexible receptor to combat a disease. This presentation will show some examples of applications made in recent time.

Effect of inertia on evasion and pursuit dynamics of prey swarms

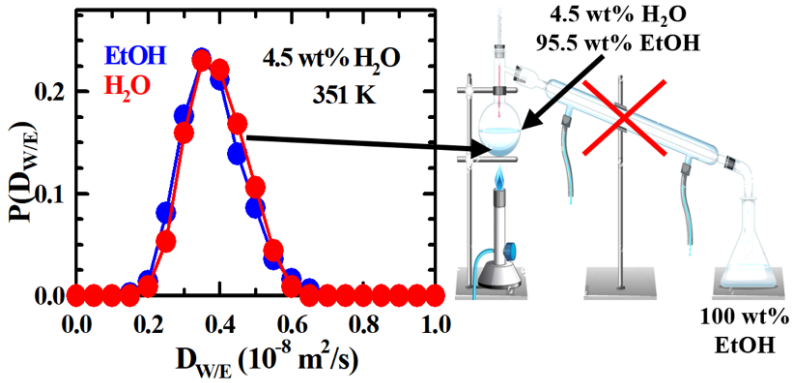
Rumi De
Indian Institute of Science Education and Research, Kolkata

Cohesive group formation has been observed in diverse species, such as a flock of birds, a school of fishes, and a swarm of insects. In nature, swarming behavior has generally been found in search of food, for breeding, to avoid predators, etc. It is quite intriguing how a large number of individuals self-organize to form collective groups and generate complex organized patterns. In this talk, I will discuss, using a simple prey-predator model, how inertia could play a pivotal role in the survival dynamics of a prey swarm being pursued by a predator. Our study shows that the varying mass of the prey and the predator strongly influences the trajectory of the prey. As seen in nature, diverse escape patterns emerge, such as circling, chasing, maneuvering into an arc, dividing into subgroups, and merging again into a single group to avoid the predator attack. Interestingly, our study reveals the existence of three distinct regimes based on the predator-to-prey mass ratio: (i) frequent chase and capture leading to the non-survival of the prey swarm, (ii) the survival regime without the capture of prey, and (iii) an intermediate regime where competition between pursuit and capture occurs, resembling an arms race as seen in natural ecosystems.

What Dictates Azeotrope Formation?

Pradip Kumar Ghorai
Indian Institute of Science Education and Research, Kolkata

What selects azeotropic pairs and governs the azeotropic condition (composition and temperature) is an open and intriguing question. The simulation studies presented here investigated this by considering ethanol-water mixtures, one of the most commonly used and widely studied binary mixtures. We find identical distributions of centre-of-mass diffusion coefficients for ethanol and water molecules in ethanol-water binary mixtures at the azeotropic condition. Moreover, the particle displacements show strong interspecies correlations at the azeotropic condition Interestingly, simulated reorientation time distributions of ethanol and water molecules become identical at the azeotropic temperature (T azeo) but at a composition different from that at which the translational diffusion distributions overlapped. Cluster analysis results clearly indicate solution structural changes as the azeotropic mixture composition is approached at T azeo . Higher order correlation also observed at the azeotropic composition.



Enigma of two-dimensional melting in a disordered environment

Amit Ghosal
Indian Institute of Science Education and Research, Kolkata

We will present our study of melting in a two-dimensional system of classical particles with Gaussian-core interactions in disordered environments. The clean system validates the conventional two-step melting with a hexatic phase intervening between the solid and the liquid. This picture gets significantly modified in the presence of disorder. Impurities in the form of a random distribution of pinning centers, forces a hexatic-like low-temperature phase extends up to T=0, which transits into the liquid at a single melting temperature T_RP. In contrast, pinning centers located at randomly chosen sites of a perfect crystal of the clean system anchor a solid at low temperatures, which undergoes a direct transition to the liquid at T_CP. Thus, the two-step melting is lost in either case of disorder. Addressing dynamics across melting, we will demonstrate intriguing signatures of cooperative motion of particles in string-like paths are found at low temperatures. Such motional footprints are common to glasses and supercooled liquids but we realize them in equilibrium dynamics, even in a pure system. Their repercussions on various spatio-temporal correlations will also be discussed.

Spectral properties of β ensemble

Anandamohan Ghosh
Indian Institute of Science Education and Research, Kolkata

The signature of quantum chaos is often related to the energy level repulsion in random matrix ensembles where the degree of repulsion is called the Dyson's index, β. We study the spectral properties of an ensemble of tridiagonal matrices, isospectral to random matrices, where β can be varied continuously to reproduce a chaotic-integrable transition. We show that the inhomogeneity in β ensemble results in the existence of Non-Ergodic Extended (NEE) states resembling Many-Body Localization (MBL) in physical systems. Interestingly, β ensemble provides a counter-example to Mott's argument that extended and localized states cannot exist simultaneously.

Cholesterol alters the kinetics and statistics of pore formation in the phospholipid membrane induced by an antimicrobial peptide

Sanat Karmakar
Jadavpur University

NK-2, an antimicrobial peptide, has emerged as a promising candidate for peptide antibiotics. In contrast to classical antibiotics, antimicrobial peptides target bacterial membranes, create defects, and eventually disintegrate the membrane by forming the transmembrane pores. However, a complete understanding of the mechanisms of cellular apoptosis and the molecular basis of membrane selectivity is still in dispute. In the present study, we have shown that cholesterol significantly modulates NK-2-induced transmembrane pores on negatively charged phospholipid membranes. The kinetics and statistics of pore formation were determined from the analysis of phase contrast micrographs of giant unilamellar vesicles. Further, significant interaction of NK-2 with anionic membranes has been envisaged based on zeta potential and dynamic light scattering. The binding free energy and effective peptide charge have been delineated using a theoretical approach. The present biophysical study will help us to understand the effect of cholesterol on the antimicrobial activity of the membrane, which eventually provides important insights into the development of peptide antibiotics.

Hyperuniformity in Ashkin-Teller model

Pradeep K Mohanty
Indian Institute of Science Education and Research, Kolkata

We show that equilibrium systems in d dimension that obey the inequality $d\nu > 2$, known as Harris criterion, exhibit hyperuniform energy fluctuations in their critical states. Ashkin-Teller model is an example in $d = 2$. Point configurations generated by deleting sites that has coarse-grained energy below a threshold also exhibit suppressed number fluctuations.

Comparing networks: Lessons for biology, mutations, and, phage resistance in bacteria

Soumen Roy
Bose Institute

Differentiating between two (nearly) indistinguishable graphs with a set of common or identical nodes and identifying the implications therefrom, is an important yet rather neglected problem in the statistical physics of networks. Using rigorous mathematical methods, we propose a new measure called shortest path alteration fraction (SPAF) to compare any two networks. We demonstrate how our measure successfully captures reported effects of well-studied mutations and predicts new ones in five diverse microbial species, each from a different taxon. We experimentally generate a mutant of Mycobacterium smegmatis, mc2155, which is resistant to the mycobacteriophage D29. Extensive characterisation of this mutant presents significant phenotypic alterations. We exhibit the general effectiveness of our measure by illustrating how it unravels connections between mutations and the resulting phenotypes.

Enzyme Assembly and Microscopic Gyration

Arnab Saha
Calcutta University

Metabolism is crucial for cellular life to survive. It encompasses sequential biochemical reactions and processes. The rate of the reactions are controlled and facilitated by catalysts called enzymes. These enzymes, instead being well-mixed throughout the cell, often reside in supramolecular assemblies (e.g. ribosomes, microtubules, contractile systems etc.) as enzyme complexes. Recently it is being discussed that diffusion and kinetic asymmetries that causes non-reciprocal interactions among the sequential enzymes facilitate the formation of enzyme complexes. In this talk we will discuss a possible mechanism (microscopic gyration) that may explain the role of these asymmetries in forming the enzyme complexes termed as metabolons.

Computational Modeling for Self Assembled Amphiphiles

Jayashree Saha
Calcutta University

Modeling of coarse grained potential for amphiphatic molecules in aqueous solution will be discussed.

Site and bond percolation in distorted lattices in two and three dimensions

Ankur Sensharma
University of Gour Banga

We have studied a new mechanism of percolation in distorted square, triangular, and simple cubic lattices, where the sites are randomly but controllably shifted from their regular positions by small amounts. When usual neighbourhood is considered, the site percolation threshold p_c always increases with distortion. This means, spanning becomes difficult with distortion. However, if a more flexible neighbourhood, owing to distortion, is considered, the variation of p_c is not monotonic. One can also define a connection threshold as the maximum allowed distance between the sites to form a bond. Not surprisingly, p_c decreases as connection threshold increases. The bond percolation shows similar variation of percolation threshold p_b on distortion. In this case, it is possible to determine a critical connection threshold below which no spanning is possible. Evaluation of the critical exponents shows that the distortion of the lattices does not chage the universality class of the percolation transition.

Fragility in Glassy Liquids: A Structural Approach Based on Machine Learning

Indrajit Tah
CSIR-CGCRI

The rapid growth of viscosity or relaxation time upon supercooling is universal hallmark of glassy liquids. The temperature dependence of the viscosity, however, is quite non-universal for glassy liquids and is characterized by the system's "fragility," with liquids with a nearly Arrhenius temperature-dependent viscosities referred to as strong liquids and those with strongly super-Arrhenius behavior referred to as fragile liquids. What makes some liquids strong and others fragile is still not wellunderstood. Here we explore this question in a family of glassy liquids that range from extremely strong to extremely fragile, using "softness," a structural variable identified by machine learning to be highly correlated with dynamical rearrangements. We use a support vector machine to identify softness as a linear combination of structural quantities, and show that the same linear combination is successful in predicting rearrangements across the entire family of glassy liquids. We find that fragility is reflectedin the softness-dependence of energy barriers.

Dynamic fluctuations in systems with broken time-reversal symmetry and centre-of-mass conservation

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