Recent Topics on Statistical Mechanics

Abstract Booklet

11-13 December, 2019

National Institute of Science Education and Research, Bhubaneswar

Talk Abstracts

Wednesday
Date : 11/12/2019

Time : 10.00 am - 10.50 am

Hydrodynamic description of one-dimensional Hamiltonian systems

Abhishek Dhar
ICTS, Bangalore

The talk will describe work describing our understanding of dynamical correlations in a large class of one-dimensional systems using the framework of nonlinear fluctuating hydrodynamics. Numerical results on anharmonic oscillator chains and spin systems will be presented.

Time : 11.15 am - 11.45 am

Chaotic orbits of ellipsoids in fluid

Rama Govindarajan
ICTS, Bangalore

There is a theorem of Kozlov and Onishchenko which states that the motion of an ellipsoid of rotation in inviscid fluid is integrable. We investigate (a) what happens to triaxial ellipsoids and (b) ellipsoids of rotation in viscous fluid. We show chaos in these dynamics and also discuss the dynamics in various limits.

Work done with: Erich Essmann, Pei Shui and Prashant Valluri.

Time : 11.45 am - 12.15 pm

Interface growth driven by a single active particle*

Mustansir Barma
TIFR, Hyderabad

Active particles on an interface define a simple model for energy-consuming proteins embedded in the plasma membrane of a cell, responsible for membrane deformation and cell movement. We study pattern formation, fluctuations and scaling induced by a single active walker on an initially flat static interface. A puller changes local valleys into hills, simulating growth, while itself sliding and seeking new valleys. Our numerical simulations reveal that in 1D: (a) The mean interface assumes a tent-like profile, whose breadth and height grow as power laws in time. The growth, dynamic and roughness exponents are found to be 2/3, 3/2 and 12 respectively implying a breakdown of customary Family-Vicsek scaling. (b) Puller motion is superdiffusive in the transverse direction, as it pulls the interface upwards. The probability distribution of displacement is bimodal. For a puller on a static 2D interface, the distribution of displacement and mean profile also obey scaling. Finally, we show that a pusher on a fluctuating interface moves subdiffusively.

Time : 12.15 pm - 12.45 pm

Martingale theory for housekeeping heat

Shamik Gupta
RKMVERI, Kolkata

The housekeeping heat is the energy exchanged between a system and its environment in a nonequilibrium process and is a result of the violation of detailed balance. We describe fluctuations of the housekeeping heat in mesoscopic systems using the theory of martingales, a mathematical framework widely used in probability theory and finance. We show that the exponentiated housekeeping heat (in units of k_{BT}, with k_B the Boltzmann constant and T the temperature) of a Markovian nonequilibrium process under arbitrary time-dependent driving is a martingale process. From this result, we derive universal equalities and inequalities for the statistics of stopping times and suprema of the housekeeping heat. We test our results with numerical simulations of a system driven out of equilibrium and described by Langevin dynamics.

Time : 12.45 pm - 1.00 pm

The elusive connection between structure and dynamics in the supercooled liquids

Sarika Maitra Bhattacharyya [1]
CSIR, NCL

In theories of liquids the structure provides information of the thermodynamic and dynamic quantities. However in supercooled liquid although the dynamics changes over orders of magnitude the change in structure is small and this observation raises the question about the role of structure in the dynamics. Studies showing that two systems which have very similar structure have orders of magnitude difference in dynamics at low temperatures further strengthens the argument that pair structure does not play any role in the slowing down of the dynamics. The common wisdom in supercooled liquid community is that many body correlation drives the slowing down of the dynamics . Based on our work I will present a completely new and counter intuitive understanding about the role of pair and higher order correlations in the dynamics. We find that slow dynamics in supercooled liquid is driven by the pair correlation and many body correlation helps the system to explore larger phase space and speed up the dynamics[1]. I will also present a recently developed mean field theory and show that the information of the well known dynamical transition temperature is embedded in the pair structure of the liquid[2]. Motivated by our work in a recent study a softness parameter was described which is a weighted integral of the structure where the weight is obtained from the dynamics using machine learning (MI)[3]. The study shows that for systems having similar structure this softness varies and the dynamics for two systems when plotted against the softness shows a master plot (Fig.1b). We now show from our mean field theory that indeed the mean field potential of the two systems have different softness which can describe the difference in the dynamics (Fig.1a) thus giving the softness parameter obtained from MI a physical meaning[4].

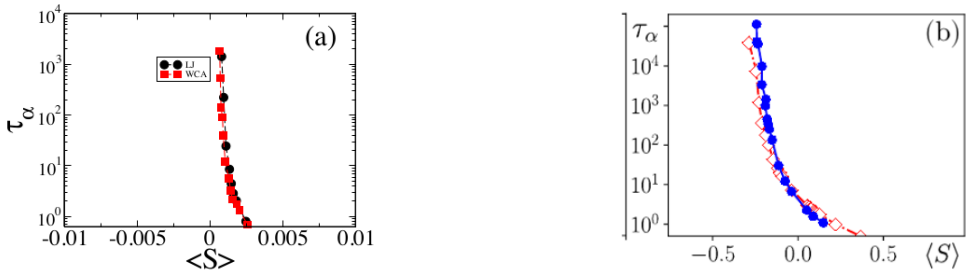

Fig1. The relaxation time vs. softness parameter,$< S >$ (a) $< S >$ from mean field theory [4] (b) $< S >$ from Machine learning [3]

[1]A. Banerjee, S. Sengupta, S. Sastry, and S. M. Bhattacharyya. Phys. Rev. Lett., 113, 225701 (2014). [2] M. K. Nandi, A. Banerjee, C. Dasgupta and S. M. Bhattacharyya Phys. Rev. Lett., 119, 265502 (2017). [3] F. P. Landes, G. Biroli, O. Dauchot, A. J. Liu, and D. R.

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Reichman, arXiv:1906.01103v1. [4] M. K. Nandi, I. Saha, C. Dasgupta and S. M. Bhattacharyya (Ms. under preparation).

Time : 2.30 pm - 3.20 pm

Sriram Ramaswamy
IISc, Bangalore

TBA

Time : 3.20 pm - 3.50 pm

Glassy Dynamics in Dense Active Matter

Rajesh Ganapathy
JNCASR, Bangalore

The glass transition – wherein flowing liquids transform into rigid solids without an apparent change in structure – is well-studied for systems in thermal equilibrium [1]. In the past decade, numerous studies have pointed out that many of the phenomena associated with glassy slowing down for systems in thermal equilibrium are also observed in systems where fluctuations do not have a thermal origin – prototypical examples being active granular matter and living matter [2]. These systems are inherently out-of-equilibrium as there is a continuous input of energy at the particle scale and detailed balance is violated, therefore. Simulations have found that activity introduces new modes of relaxation and thereby speeds up liquid dynamics in a manner that has no parallels in equilibrium supercooled liquids [3-5]. Many of these predictions are yet to be observed and quantified in experiments. In my talk, I will describe results from recent active granular matter experiments at high densities that attempts to address these open issues.

1. Berthier, L., Biroli, G. (2011). Theoretical perspective on the glass transition and amorphous materials. Reviews of Modern Physics, 83(2), 587.
2. Glass-like dynamics of collective cell migration. Proceedings of the National Academy of Sciences, 108(12), 4714-4719.
3. Berthier, L., and Kurchan, J. (2013). Non-equilibrium glass transitions in driven and active matter. Nature Physics, 9(5), 310-314.
4. Berthier, L. (2014). Nonequilibrium glassy dynamics of self-propelled hard disks. Physical review letters, 1 12(22), 220602.
5. Nandi, S. K., Mandal, R., Bhuyan, P. J., Dasgupta, C., Rao, M.,amp; Gov, N. S. (2018). A random First- order transition theory for an active glass. Proceedings of the National Academy of Sciences, 115(30),7688-7693.

Time : 3.50 pm - 4.05 pm

Role of architecture and topology in the scaling behaviour of sparsely-grafted nanoparticles

Md Moinuddin, Mukta Tripathy [2]

IIT Bombay

Polymer grafted nanoparticles have applications in mechanically reinforced materials, drug delivery, fuel cells, gas-separation membranes, and as sensing materials. In this talk we explore the phase behaviour of sparsely-grafted nanoparticles. We use integral equation theory to determine the structure and phase behaviour of polymer-grafted nanoparticles. We study four systems in particular: singly-grafted nanoparticles, doublygrafted nanoparticles, polymer-linked nanoparticles (polymer chains tethered to nanoparticles at each end), and ring-grafted nanoparticles (both chain ends of the polymer are tethered to a single nanoparticle).

We find that even in the absence of any chemical anisotropy, these systems can selfassemble into polymer-rich and nanoparticle rich domains. The self-assembly is driven by the shape anisotropy of the grafted-nanoparticle species, and the domain length is a complex function of both the nanoparticle and the polymer chain length. This domain length scale also shows a remarkable scaling behaviour. We determine how the phase behaviour and domain lengths depend on the architecture and topography of the polymer-grafted nanoparticle species. The phase behaviour of polymer-linked nanoparticles, singly-grafted nanoparticles, doubly-nanoparticles, and ring-grafted nanoparticles are remarkably similar. In all four cases, the transition between the homogeneous to self-assembled state are occurs at lower packing fractions as either polymer chain length or nanoparticle diameter increases. However, the scaling exponent of the domain length of is a strong function of the grafting topography. While the exponent is the same for all linear architectures, the ring-grafted nanoparticle system has a completely distinct scaling behavior.

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Time : 4.05 pm - 4.20 pm

Phase separation in a 2D binary colloidal mixture by quorum sensing activity

Jalim Singh [3]

NISER, Bhubaneswar

We present results from the Langevin dynamics simulations of a glassy active-passive mixture of soft-repulsive binary colloidal disks. Activity on the small particles is applied according to the quorum sensing (QS) scheme, developed for this study, in which a small particle will be active for a persistence time if its local nearest neighbours are equal to or greater than a certain threshold value. We start with a passive glassy state of the system and apply activity to the smaller size particles, which shows a non-monotonous continuous glassy character of the active particles with the persistence time of the active force, from its passive limit (zero active force). On the other hand, passive particles phase separate at an intermediate persistence time of the active force, resulting the system into the hexatic-liquid and solid-liquid phases. Thus, our system shows three regimes as active glass, phase separation, and active liquid as the persistence time increases from its smaller values. We show that the solid and hexatic phases consisting of passive large particles are stable due to the smaller momentum transfer from active to passive particles compared to the higher persistence time where the positional and orientational ordering vanishes. Our model is relevant to the active biological systems, where glassy dynamics is present, *e.g.*, bacterial cytoplasm [1], biological tissues [2], dense QS bacteria [3], and in the synthetic smart amorphous glasses [4].

[1] B. R. Parry *et al.*, Cell **156**, 183 (2014). [2] Dapeng Bi, Xingbo Yang, M. Cristina Marchetti and M. Lisa Manning, PRX **6**, 021011 (2016). [3] Liesbeth M C Janssen, J. Phys.: Condens. Matt. **31**, 503002 (2019). [4] Sarah A. Jung, Christine A. Chapman, and Wai-Leung Ng, PLoS Pathog. **11**, e1004837 (2015).

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Time : 4.45 pm - 5.15 pm

Asymmetric exclusion processes on an inhomogeneous ring

Abhik Basu
SINP, Kolkata

We discuss the nature of the steady states in asymmetric exclusion processes on an inhomogeneous ring. We discuss several sources of inhomogeneities including isolated point defects, smoothly varying and random quenched disordered hopping rates in the ring.

Time : 5.15 pm - 5.45 pm

Two-dimensional evaporative self- assembly of soft colloids at interfaces

Dilip K Sathpathy
IIT, Madras

The creation of self-assembled uniform monolayers of colloids at fluid interfaces and transforming them on to solid surfaces is not only crucial to fundamental science but also of utmost importance for soft nanotechnology. Here, we demonstrate a facile strategy which exploits the interface assisted self-assembly to obtain two-dimensional layers of soft colloids. Solvent-swollen submicrometer-sized hydrogel particles (microgels) with delicate hydrophobic - hydrophilic balance and sensitive to environmental conditions such as temperature/pH are used as soft colloids. The surface activity of the microgel particles, the interparticle interactions, and the kinetics of evaporation are tuned to generate a variety of novel two-dimensional structures, including monolayer coffee-rings, loosely packed uniform layers, and interconnected cell-like

patterns with extraordinary richness and diversity [1-4]. A smooth order- disorder transition in the self-assembled monolayers of soft colloids is identified

by constructing Euclidean Voronoi diagrams. The viscoelastic nature of the soft colloid laden interface probed by using multiple particle tracking passive microrheology and its dependence on the crosslinking-density of microgels will be presented. In addition, the suppression of the "coffee-ring effect" for hard colloids in presence of microgel particles and the origin of the depletion zones observed in evaporative self-assembly will be discussed in detail.

M. Mayarani et al. Nanoscale 9, 18798 (2017). [2] M. Mayarani et al. Langmuir 34, 14294 (2018). [3] M. Mayarani et al. Soft Matter 15, 4170 (2019). [4] M. Mayarani et al. Phys. Rev. E (submitted).

Time : 5.45 pm - 6.00 pm

Elasto-inertial Chains in a Two-dimensional Turbulent Flow

Rahul Singh [4]

ICTS, Bangalore

The interplay of inertia and elasticity is shown to have a dramatic impact on the transport of filamentary objects, modelled by bead-spring chains, in a two-dimensional turbulent flow. We show how elastic interactions amongst inertial beads result in a non-trivial sampling of the flow, ranging from entrapment within vortices to preferential sampling of straining regions. This behavior is quantified as a function of inertia and elasticity and is shown to be very different from free, non- interacting heavy particles, as well as inertialess chains [Picardo et al., Phys. Rev. Lett. 121, 244501 (2018)]. In addition, by considering two limiting cases, of a heavy-headed and a uniformly-weighted chain, we illustrate the critical role played by the mass distribution of such extended objects in their turbulent transport.

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Time : 6.00 pm - 6.15 pm

Crystallization of Binary Polymer Blends Studied by Dynamic Monte Carlo Simulation

Ashok Kumar Dasmahapatra[5]

Department of Chemical Engineering, Indian Institute of Technology, Guwahati, Assam, India

Polymer blends are known to be one of the exciting materials to prepare nanoscale devices via self-assembly. The thermodynamic and mechanical properties largely depend on their mutual miscibility. Miscible blends usually give single glass transition temperature, whereas immiscible blends produce two distinct glass transition temperatures. Since the components in the blend are chemically dissimilar they phase seperate via microphase separation. We report dynamic Mote Carlo simulation results on the crystallization of A/B binary polymer blends with varying composition, wherein both the components are crystallizable. We model A-polymer as high melting component and hence its crystallization precedes the crystallization of B-ploymer upon cooling from a homogeneous melt. The morphological development is controlled by the interplay between crystallization driving force(attractive) and de-mixing energy (repulsive) between the components. With increasing the composition of B-polymer, macrophase separation, crystallization and lamellar thickness follow a non-monotonic trend. This non-monotonic trend is attributed to the composition-heterogeneity in the blend. When one component is relatively less compared to the other, its mobility is reduced affecting transition temperature during crystallization. As a result, transition happens at a relatively low temperature (viz. enhanced thermal driving force). Isothermal crystallization reveals that the crystallization behavior and crystal morphology strongly depends on the mode of cooling. Two-step , compared to on-step isothermal crystallization provides a better crystalline structure. Finally, some recent results on the thin film crystallization on patterned substrate will be discussed. The presence of an active surface exhibits a non-intuitive crystallization trend.

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Time : 5.45 pm - 6.00 pm

Early time dynamics in the Light-Heavy Model

Samvit Mahapatra [6]

TIFR, Hyderabad

We study the early time dynamics and onset of instabilities in a non- equilibrium lattice model known as the Light-Heavy (LH) model. This system consists of two species of particles (light and heavy) advecting on a fluctuating surface (described by tilt fields). The dynamics of particles and tilts are coupled through update rules, and lead to different phases depending on their microscopic rates. We propose a local correlation function (S) that is able to distinguish between several phases of this system through its coarsening properties. Starting from a random initial configuration, S displays an initial linear rise, a broad maximum, followed by a gradual decay which could include a power-law regime. Focusing on the early time dynamics, we posit coupled evolution equations governing the densities and tilts, which at short times are well approximated by a linear set of equations. We analytically solve these equations in continuum as well as on a lattice. The predicted early time evolution of S corresponds well with direct simulations of the LH model at early times. Beyond a timescale set by an ultraviolet (lattice) cutoff and preceding the onset of coarsening, our linearised theory predicts the existence of an intermediate diffusive (power-law) regime, which we also find in simulations of the unstable regime in the LH system.

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Thursday
Date : 12/12/2019

Time : 10.00 am - 10.50 am

Active Matter at High Densities

Chandan Dasgupta
IISc and ICTS, Bangalore

In several biological systems, such as bacterial cytoplasm, cytoskeleton-motor complexes and cell nuclei, self-propulsion or activity is found to fluidize a glassy state that exhibits characteristic glassy features in the absence of activity. Recent experiments on dense systems of Janus colloids have provided a lot of information about how activity affects the colloidal glass transition.To develop a theoretical understanding of these non-equilibrium phenomena, we have studied, using molecular dynamics and Brownian dynamics simulations, the effects of activity in several model glass-forming liquids.The activity in these systems is characterized by two parameters: the active force and its persistence time. If the persistence time is short, then the observed behaviour is similar to that near the usual glass transition. The introduction of activity reduces the glass transition temperature and the glass transition disappears beyond a threshold value of the activity. Some of the effects of activity on the dynamics in the liquid state are determined by an "active temperature" that adds to the bath temperature.This can be understood from a generalization of the Random First Order Transition (RFOT) theory of the glass transition to active systems. In the limit of infinite persistence time, the fluid jams at a critical threshold as the propulsion force is lowered, with stresses concentrated along force chains. For large but finite persistence times, the approach to dynamical arrest at low propulsion force goes through a phase characterized by intermittency. This intermittency is a consequence of long periods of jamming followed by bursts of plastic yielding associated with Eshelby deformations, akin to the response of dense amorphous solids to an externally imposed shear. Thus, dense active matter brings together the physics of glass, jamming and plasticity in an internally driven classical system.

This work was carried out in collaboration with Rituparno Mandal, Pranab Jyoti Bhuyan, Pinaki Chaudhuri, Saroj Kumar Nandi, Nir Gov and Madan Rao.

Time : 10.50 am - 11.20 am

Yielding of amorphous solids: effect of pinning

Pinaki Chaudhuri

IMSc, Chennai

Amorphous solids are ubiquitous in our daily life, and their yielding behaviour is harnessed in diverse applications or significant for natural phenomena. However, till today, a systematic understanding of microscopic processes that lead to yielding, is still missing In that context, we probe the yielding response of a model amorphous material having inclusions in the form of randomly pinned particles. We show that, with increasing pinning concentration, the plastic activity becomes more spatially localized, resulting in smaller stress drops, and a corresponding increase in the magnitude of strain where yielding occurs. We demonstrate that, unlike the spatially heterogeneous and avalanche led yielding in the case of the unpinned glass, for the case of large pinning concentration, yielding takes place via a spatially homogeneous proliferation of localized events.

Time : 11.45 am - 12.15 pm

Domain Growth in Disordered Systems

Sanjay Puri
JNU, Delhi

Consider a system which is rendered thermodynamically unstable by a sudden change of parameters, e.g., temperature, pressure, etc. The system evolves towards its new equilibrium state via the emergence and growth of domains enriched in the preferred phases. We have a good understanding of domain growth in pure systems. However, most experimental systems contain both mobile and immobile impurities. We will discuss our recent work, which has demonstrated that the presence of quenched disorder leads to trapping of domain walls. The subsequent activated dynamics over disorder barriers gives rise to a logarithmic domain growth law.

Time : 12.15 pm - 12.45 pm

Velocity distribution of driven granular gases

Rajesh Ravindran
IMSc, Chennai

The velocity distribution of a gas in thermal equilibrium is known to be a gaussian with a width proportional to temperature. What is the velocity distribution of an inelastic gas driven to a steady state through external driving? This question is central to the kinetic theory of driven granular systems. It is generally accepted that the velocity distribution, counterintuitively, decays slower than a gaussian, in particular $ln[P(v)] \ -av^{3/2}$. In this talk, I will review experimental, theoretical and numerical data supporting/against this result. I will then present an exact solution of a simple microscopic model for a driven inelastic gas whose conclusions for the velocity distribution run counter to the generally accepted results.

Time : 12.45 pm - 1.00 pm

Far out-of-equilibrium dynamics of a model glass-former in 2D

Shiladitya Sengupta [7]
IIT, Roorkee

Glasses are out-of-equilibrium states of matter with liquid-like structure but solid-like rigidity and extremely slow dynamics. While the nature of dynamics is continuous in equilibrium liquids, it shows avalanche-like intermittent behaviour far out of equilibrium. Motivated by recent observations which suggest a possible mechanical origin to this behaviour, we analyze the inter-particle force network in a model glass-former. Force networks are hallmarks of a-thermal amorphous solids and are thought to be responsible for giving mechanical rigidity. In our thermal system, we find that at high enough densities, an increasingly long-lived force network emerges upon cooling and its dynamics captures structural relaxation both in and out of equilibrium.

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Time : 2.30 pm - 3.00 pm

Simulations of fluid membranes undergoing material exchange

P B Sunil Kumar
IIT, Palakkad

Intracellular organelle membranes exhibit a wide variety of morphologies that are believed to be crucial for their function. Though the organelle morphologies are dynamic, as the membranes continuously exchange materials with their environment through trafficking, they are able to maintain a characteristic steady state shape. While several molecular players responsible for generating local shape changes have been identified, the mechanisms governing the stabilization of large scale morphologies are not clearly understood. Dynamic Triangulation Monte Carlo (DTMC) is a useful technique to analyze arbitrarily shaped fluid membranes at the mesoscopic length scales. We present a modified DTMC simulation method to investigate the role of curvature generating proteins and active material exchange processes on the steady state morphology of vesicles. The role of membrane recycling processes in controlling the vesicle morphology and in stabilizing compositional inhomogeneity on the vesicle surface is discussed.

Time : 3.00 pm - 3.30 pm

Visualising yielding of amorphous solids using colloidal suspensions

Vijayakumar Chikkadi
IISER, Pune

Amorphous solids when subject to an external stress exhibit linear elastic behavior up to a critical strain beyond which the response becomes nonlinear, indicating the onset of plastic flow. Such macroscopic measurements are very common in engineering and rheological applications. However, the microscopic physics that governs the onset of yielding, where a material changes its shape permanently under external deformation, has remained elusive. In this talk I will present experimental results on sheared colloidal glasses that will shed new light on yielding of amorphous solids. Our results reveal that clusters of non-affine deformation grow and percolate on approach to yielding. We establish the robustness of our results by comparing them to simulations. I will also highlight some recent results on structural changes accompanying this transition.

Time : 3.30 pm - 4.00 pm

Tuning of friction noise by accessing the rolling-sliding option

Shankar Ghosh
TIFR, Mumbai

Pulse width modulation technique (PWM) is a versatile and a common way to control power transmission in electrical systems. However, its mechanical analogue is far from being that versatile. This point is best illustrated by using the particular example of automotive vehicles where friction plates are used for clutching and braking purposes. If a sudden brake is to be applied, it is preferable that the coupling between the brake pads and the inner rim of the wheel is strong. Similarly, for maximum force transmission, the clutch should strongly couple the gearbox to the engine. However, when caught up in traffic while driving uphill, one often uses a technique called feathering the clutch where a driver gets better control over the vehicle by alternately pressing and releasing the brake or clutch which makes the frictional coupling time-varying(noisy). In essence, there are situations which may demand a mechanical system to exhibit strong frictional coupling in one instance of time and weak frictional coupling in another instance. This is commonly achieved by making the coupling noisy where the system is constantly made to toggle between states which have strong (e.g. brakes on) and weak (e.g. brakes off) friction. Though operatively it appears to be similar to PWM, the presence of inertial forces and continuous fretting makes this general principle of controlling the power transmission by varying the duty cycle more difficult to implement as compared to its electrical analogue. I will talk about ways in which the complexity that arises from the third body frictional interactions of balls sandwiched between the surfaces can be harnessed in order to continuously tune the noise in the frictional coupling.

Time : 4.00 pm - 4.15 pm

Tumbling of polymer in multi-gradient field and its kinetics

Sadhana Singh [8]
BHU, Varanasi

We study the classic problem of dynamical evolution of a polymer in a shear flow. Interestingly, the polymer goes through several distinctly identifiable conformations, during its passage from coiled to stretched states back and forth. We identify these conformations assumed by the polymer while tumbling, and study the kinetics of the process in terms of the residence and recurrence times of individual conformations. The distribution of residence times exhibit exponentially decaying tails which helps us build an effective Markovian picture, of the truly non-Markovian problem. We present the explicit W-matrix for the coarse-grained evo- lution via a Master equation, and study its elements as a function of Weissenberg number. We show that the time-scales of decay of the au- tocorrelation function for the full Langevin dynamics, compare quite well with the approximate results from the Master equation approach.

[1] Sadhana Singh, R. K. Singh, Dibyendu Das, and Sanjay Kumar, Physical Review E 99, 030501(R) (2019).

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Time : 4.15 pm - 4.30 pm

Origin of the long-ranged attraction or repulsion between intruders in a confined granular medium

Anki Reddy Katha [9]
IIT, Guwahati

Few studies demonstrated that there exists a long-ranged force between intruders placed at a certain distance from each other in granular flow. The origin of these long-ranged forces induced collectively by the grains has not been fully understood. In our work, we provide a unified explanation for the origin of both attraction and repulsion between two intruders in terms of the building up of force chains and their subsequent buckling. The surface and shear zone of the other intruder has a significant contribution to the strength or buckling of the force chains. Bernoulli's effect used in earlier studies predicts the nature of these forces, viz., attraction or repulsion, correctly but is not well-supported as observed in our study. The time-averaged flow fields around the intruders also support our explanation for the origin as evidenced by the burst in kinetic energy and granular temperature. The model proposed in this work predicts the qualitative trend of the sideways force with the separation between the intruders by combining Bernoulli's equation with minimum contact criterion of force chains. There exists an equilibrium at which the intruders neither attract nor repel each other and a certain separation distance where maximum attraction occurs between the two intruders. The effects of the static pressure, the velocity of the moving intruders, and the friction coefficient on the attraction or repulsion force between the intruders have also been explored in our system.

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Friday
Date : 13/12/2019

Time : 9.30 am - 10.20 am

Madan Rao
NCBS, Bangalore

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Time : 10.20 am - 10.50 am

Shachi Gosavi
NCBS, Bangalore

Vignettes in protein design.

Time : 10.50 am - 11.05 am

Propulsion at small length scale: in pursuit of biomimetic synthetic motors

Snigdha Thakur [10]

IISER, Bhopal

Internal conversion of chemical energy to mechanical energy leading to self- propulsion at small length scale is widespread in nature. One promising example for the same is biological nanomotors that play an essential role in transporta- tion within cell. In addition to these biochemical motors, synthetic molecular motors have been designed that employ chemical, light or other energy sources to perform directed motion. Many of the applications of such motors centre around issues concerning cargo transport and navigation in channels. However, the combination of low Reynolds number and thermal fluctuations that makes the direct propulsion at small length scale very difficult. In order to achieve effective directed propulsion at those length scale without any external inter- vention, it is important to devise strategies that can help the nanomotors to overcome the challenge imposed by thermal fluctuations. A model for the synthetic motor where swimming is powered by asymmetrical chemical reactions on its surface will be discussed. The propulsion properties of such motors can be altered if the environment in which they move is chemically active. Dynamics of both rigid and non-rigid self-propelled nanomotors in chemically active and inactive media and their collective dynamics will also be analysed.

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Time : 11.30 am - 12.00 pm

Anomalous diffusion of randomly migrating eukaryotic cells

Manoj Gopalakrishnan
IIT, Madras

Chemotaxis is a common mode of motility found in both prokaryotic and eukaryotic cells, by which a cell tries to follow a chemical gradient upstream or downstream. While prokaryotic bacteria like E.coli measure the chemical environment by performing a "run and tumble" walk, eukaryotic cells "polarise" when exposed to an external gradient by non-uniform localisation of intracellular signaling molecules. Generation of this internal polarity vector, or "chemical compass", guides the motion of the cell by its coupling to actin polymerisation. Interestingly, in the absence of a chemo-attractant gradient, many eukaryotic cells have been found to move about randomly in a super-diffusive manner, characterised by long-range correlations in velocity. Using a rather generic model of cell polarisation, we argue that the origins of this super-diffusive motion might lie in the slow, algebraic decay of auto-correlation of the cell polarity, which can be traced to spontaneous density fluctuations in an otherwise uniform chemo-attractant concentration field.

Time : 12.00 pm - 12:15 pm

Geometric signature of surface tension in 3D tissues

Preeti Sahu [11]

Syracuse University

Dense biological tissues maintain sharp surfaces between cell types performing different functions. For example, in multi-layered epithelia, the bottom-most basal layer is responsible for cell proliferation. This layer is distinctly compartmentalized from the suprabasal layer above that helps maintain structural integrity, although the mechanisms for this compartmentalization remain unclear. One possible candidate is tissue surface tension, which contributes to cell sorting and compartmentalization in embryonic development. Here, we use computational models to identify experimentally accessible signatures of tissue surface tension between two distinct layers in a fully 3D simulation. We find that cells adjacent to a boundary with tissue surface tension exhibit several distinct features, including a bimodal distribution of facet areas along the boundary and a clear change in overall cell shape consistent with nematic- like ordering along the boundary. The magnitude of these geometric cell shape changes scales directly with the magnitude of the tissue surface tension, suggesting that experiments might estimate the magnitude of surface tension simply by segmenting a 3D tissue. As a next step, we will investigate how proliferating cells in the basal layer are able to push into the layer above in spite of the mechanical barrier in between.

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Time : 12.15 pm - 12:30 pm

DNA in confined geometry

Navin Singh [12]

BITS Pilani

DNA inside the cellular environment works in a confined space. Depending on the confinement, the dynamics and interaction of bio-molecules changes. Intense research of the transcription and replication of DNA in the confined state is structurally significant to understand the self-assembly of DNA in a chamber or channel. We consider double-stranded DNA (dsDNA) molecules of different length and sequence and study the thermal stability of the molecule in a confined space of different geometries. We use a statistical model and evaluate the melting profile of DNA in conical as well as cylindrical geometries. Our results show that not only the confinement but also the geometry of the confined space plays a prominent role in the stability and opening behaviour of the molecule.

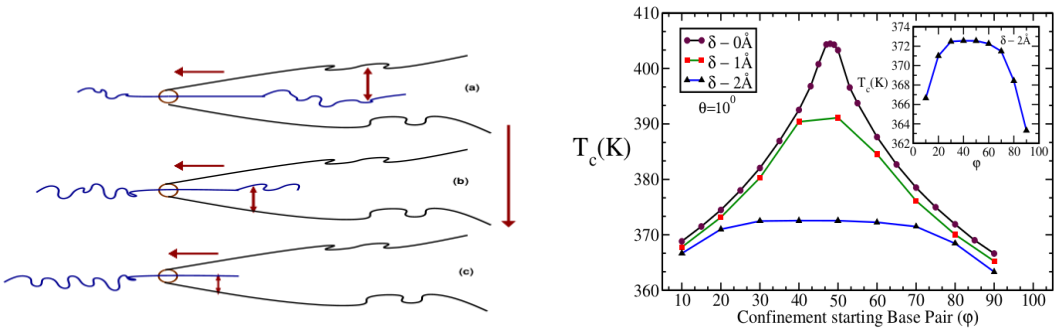

Figure 1: FIG. 1. (On left) The schematic of translocation process. (On right) The variation in the transition temperature of DNA of 100 base pairs with a fraction outside the conical cell for different angular separations.

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Time : 12.30 pm - 12:45 pm

Molecular dynamics simulation study of possible inhibitory effects of choline-based co-solutes on the aggregation tendencies of the toxic core of the Parkinson's causing protein, -synuclein

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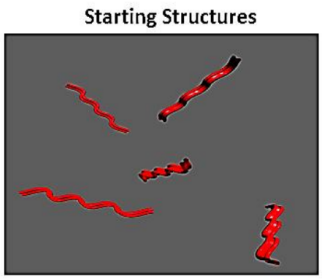
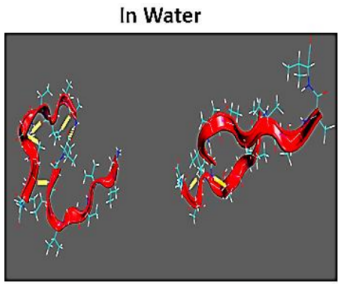
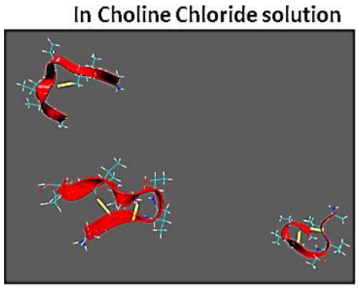
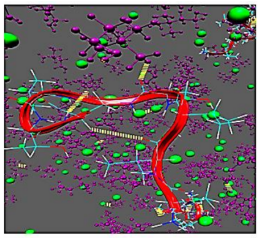
The common neurodegenerative disorder, Parkinson's disease is associated with lesions called Lewy bodies, in degenerating neurons, that are composed of aggregates of -synuclein protein. 1–3 This protein is also involved in the pathogenesis of diseases like multiple system atrophy and Alzheimers' disease. Unfortunately, there has been a lack of definitive solutions to target the formation of such fibrils/oligomers through medication/treatment. Choline based co-solutes in form of osmolytes or ionic liquids are not only bio-compatible but are also rapidly gaining attention due to their abilities to prevent aggregation as well as denaturation of proteins. 4–7 . In the present study, all-atom classical molecular dynamics simulations have been carried out to investigate the solvation behavior as well as aggregation tendencies of the fibril forming toxic core of synuclein or NACore, the structure of which has been recently unearthed through cryo-EM spectroscopy. 8 We considered the effects of different choline-based co-solutes viz. choline chloride, choline O-sulfate, and various amino acid based ionic liquids with anions like glycinate, prolinate, arginate and aspartate.









Choline Chloride (cation in purple and anion in green) around the peptide

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Figure: Snapshots from the simulation trajectory showing the initiation of aggregates in the NACore in water (from as early as 5-15 ns, while the aggregation is suppressed in 1m ionic liquid. Interaction of IL with the peptide may influence the process.

The simulations were carried out using both AMBER99SB-ILDN as well as CHARMM27 force fields as present in the GROMACS (5.1.4) package, with the total runtime in the micro-second scale. The properties evaluated ranged from radial distribution functions to hydrogen bond structural relaxation rates along with conformational changes gauged from trajectory snapshots, secondary structure analysis, radius of gyration, root mean square fluctuations and solvent accessible surface area. The propensity of the different conformations sampled was obtained from cluster analysis. It was found that fibrillation tendencies begin to dominate pretty early in the simulation time-scale in pure water whereas inhibitory effects (of varying degrees) were seen in the presence of the choline-based co-solutes. It was seen that the co-solutes had varying modes of action such as interacting directly with the peptide backbone as well as with non-polar side chains or by modification of the water solvation structure in the solution. The resultant effect is not only interference with the inter-peptide hydrogen bonding but also suppression of transformation into the beta-sheet conformations. We are presently also employing umbrella sampling methods to calculate the potential of mean force between the peptides. This study is being presently extended to see which of these co-solutes could destabilize the pre-formed protofibrils (with/without presence of agents like urea).

(1) Baba, M.; Nakajo, S.; Tu, P.-H.; Tomita, T.; Nakaya, K.; Lee, V. M.; Trojanowski, J. Q.; Iwatsubo, T. Aggregation of Alpha-Synuclein in Lewy Bodies of Sporadic Parkinson's Disease and Dementia with Lewy Bodies. Am. J. Pathol. 1998, 152 (4), 879. (2) Parihar, A.; Parihar, P.; Solanki, I.; Parihar, M. S. Alpha Synuclein and Parkinson's Disease. In Pathology, Prevention and Therapeutics of Neurodegenerative Disease; Springer, 2019; pp 1–14. (3) Lücking, C. B.; Brice, A. Alpha-Synuclein and Parkinson's Disease. Cell. Mol. Life Sci. CMLS 2000, 57 (13–14), 1894–1908. (4) Hagihara, M.; Takei, A.; Ishii, T.; Hayashi, F.; Kubota, K.; Wakamatsu, K.; Nameki, N. Inhibitory Effects of Choline-O-Sulfate on Amyloid Formation of Human Islet Amyloid Polypeptide. FEBS Open Bio 2012, 2, 20–25. (5) Paul, S.; Paul, S. Molecular Dynamics Simulation Study on the Inhibitory Effects of Choline-O- Sulfate on HIAPP Protofibrilation. J. Comput. Chem. 2019. (6) Kumar, A.; Venkatesu, P. Innovative Aspects of Protein Stability in Ionic Liquid Mixtures. Biophys. Rev. 2018, 10 (3), 841–846. (7) Kumar, A.; Bhakuni, K.; Venkatesu, P. Strategic Planning of Proteins in Ionic Liquids: Future Solvents for Enhanced Stability of Protein against Multiple Stresses. Phys. Chem. Chem. Phys. 2019. (8) Rodriguez, J. A.; Ivanova, M. I.; Sawaya, M. R.; Cascio, D.; Reyes, F. E.; Shi, D.; Sangwan, S.; Guenther, E. L.; Johnson, L. M.; Zhang, M.; et al. Structure of the Toxic Core of -Synuclein from Invisible Crystals. Nature 2015, 525, 486.

Time : 12.45 pm - 1:00 pm

On the Question of Ergodicity in Quantum Spin Glass Phase and its role in Quantum Annealing

Sudip Mukherjee [14]

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We have studied the critical behavior of quantum Sherrington-Kirkpatrick (SK) model at finite as well as at zero temperatures. Through the analysis of Binder cumulant we have determined the entire phase diagram of the model and from the scaling analysis of the numerical data we have obtained the correlation length exponent. For both the critical Binder cumulant and the correlation length exponent, we observe a crossover from classical to quantum fluctuation dominated values at a finite temperature. We have studied the behavior of order parameter distribution of the model in the spin glass phase (at finite and zero temperatures). Along with classical fluctuation dominated nonergodic region (where the replica symmetry is broken), we also find a quantum fluctuation dominated low temperature ergodic region in the spin glass phase. In this quantum fluctuation dominated region, the order parameter distribution gets narrowly peaked about its most probable value and eventually becomes a delta function in the infinite system size limit (indicating replica symmetry restoration or ergodicity in the system). We have also found that the annealing time (to reach a very low energy level of the classical SK model) becomes practically system size independent, when the annealing paths pass through this ergodic region. In contrast, when such paths pass through the nonergodic region, the convergence time grows strongly with the system size. We have presented a study of the auto-correlation of the spins in both ergodic and nonergodic regions. We have found significant increase in the relaxation time (also change in the relaxation behavior) in the classical fluctuation dominated (nonergodic) region, compared to that in the quantum fluctuation dominated (ergodic) region of the spin glass phase.

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Time : 2.30 pm - 3:00 pm

Improved Upper Bounds on the Asymptotic Growth Velocity of Eden Clusters

Deepak Dhar
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We consider the asymptotic shape of clusters in the Eden model on a d-dimensional hypercubical lattice. We discuss two improvements for the well-known upper bound to the growth velocity in different directions by that of the independent branching process (IBP). In the IBP, each cell gives rise to a daughter cell at a neighboring site at a constant rate. In the first improvement, we do not allow such births along the bond connecting the cell to its mother cell. In the second, we iteratively evolve the system by a growth as IBP for a duration t, followed by culling process in which if any cell produced a descendant within this interval, who occupies the same site as the cell itself, then the descendant is removed. We study the improvement on the upper bound on the velocity for different dimensions d. The bounds are asymptotically exact in the large-d limit. But, even in d = 2, the improvement over the IBP approximation is only a few percent.

Time : 3.00 pm - 3:30 pm

Dynamical Quantum Phase Transitions: A few exact results

Somendra M Bhattacharjee
Ashoka University, Sonepat

Dynamical quantum phase transitions are phase transitions in time in a large quantum system during a quench. We present a few exact results on the transition based on the analysis of zeros of the partition function and renormalization group transformations for the transverse field Ising model and the three state Potts model in one and higher dimensional scale invariant lattices.
Ref: A Khatun and SMB, PRL 123, 160603 (2019)

Time : 3.30 pm - 4:00 pm

How to train your atoms: creating order in colloids and bots by engineering displacement fluctuations

Surajit Sengupta

TIFR Hyderabad

Inducing specific kinds of translational order in a collection of colloidal particles is useful for various purposes such as obtaining fundamental insights into ordering processes, understanding the equilibrium and dynamic properties of crystals, creating optical band gap materials etc. This is usually accomplished, either by using external fields such as etched templates or crossed laser beams, or by engineering the nature of inter-particle interactions. Each of these methods have their disadvantages. While translational invariance is broken in the former, the latter method of creating particles that interact to produce tailor-made ordered structures is non-trivial, requiring complex chemistry. Also, the possible kinds of order are fixed once the interactions are.

Similarly, swarms of autonomous drones or bots are useful for many purposes such as surveying unknown territory, taking measurements of scientifically or economically important quantities over a large area, pollinating, decontaminating or simply featuring in purely decorative drone shows. In many of these applications, having the bots arranged in a specific pattern is useful. Disruption of the pattern may occur due to many factors e.g. random noise in the propulsion mechanism, atmospheric or ocean turbulence etc. Stabilising any given ordered pattern in such a swarm is energy expensive and requires extensive computation and communication overheads.

We propose an algorithm where one can set any given patterns in either colloidal particles or drones in an energy efficient way. The strategy involves suppressing a class of fluctuations viz. non-affine displacements, away from the given reference pattern while allowing affine deformations such as translations and rotations. In the first case of colloidal particles this may be done using feedback-controlled dynamic laser traps and in the second case by small, precisely directed thrusts of propulsion. One can show that the average power expended in such a stabilisation process is zero in the steady state. Additionally, we show that the act of maintaining the order or pattern under the influence of a destabilising field (thermal or turbulent) automatically imprints the statistics of this field on the "non-affine" forces. This is particularly useful for the second application where bots can extract velocity correlations of the turbulent field without actually measuring the flow velocity!

Time : 4.20 pm - 4:35 pm

The exact phase diagrams for a class of left-permeable asymmetric exclusion processes

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IISc, Bangalore

Exclusion processes are well-known prototypical models in non-equilibrium statistical physics. The open asymmetric simple exclusion process (ASEP) involves a single species of particles hopping with excluded volume interaction along an open one-dimensional finite lattice. Though the dynamical rules of evolution are simple, ASEP exhibits intriguing and complex behaviour. For example, ASEP manifests rich physical phenomena like boundary-induced phase transitions and formation of shock-waves. Besides, ASEP is an integrable model. Integrability renders ASEP amenable to exact analysis using mathematical techniques such as matrix product ansatz (due to Derrida, Evans, Hakim and Pasquier) and Bethe ansatz.

ASEP with multiple species is a natural generalization of single-species ASEP. Multispecies ASEPs are interesting also because they have applications in traffic flow, cell motility and biological systems. However, multispecies ASEP is a highly non-trivial problem. In our work, we study an integrable two-species partially asymmetric exclusion process called the left-permeable ASEP or LPASEP and its multispecies generalization, called the mLPASEP. In both these models, the left boundary is permeable to all species but the right boundary is impermeable to one of them. For the LPASEP, we construct a matrix product solution for the stationary state and thereby compute the exact stationary phase diagram for densities and currents. The phase diagram has three phases with a structure similar to the single-species ASEP. We obtain further structure in the phase diagram as we show existence of subphases by computing boundary densities of each species.

We define mLPASEP for arbitrary number of species. Then using projections onto the LPASEP, we derive densities and currents as well as the phase diagram in the steady state. One observes the phenomenon of dynamical expulsion of one or more species in most of the phases. We explain this phenomenon and the density profiles in each phase using interacting shocks.

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Time : 4.35 pm - 4:50 pm

Relaxation to equilibrium in models of classical spins with long-range interactions

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For a model long-range interacting system of classical Heisenberg spins, we study how fluctuations, such as those arising from having a finite system size or through interaction with the environment, affect the dynamical process of relaxation to Boltzmann-Gibbs equilibrium. Under deterministic spin precessional dynamics, we unveil the full range of quasistationary behavior observed during relaxation to equilibrium, whereby the system is trapped in nonequilibrium states for times that diverge with the system size. The corresponding stochastic dynamics, modeling interaction with the environment and constructed in the spirit of the stochastic Landau-Lifshitz-Gilbert equation, however shows a fast relaxation to equilibrium on a size-independent timescale and no signature of quasistationarity, provided the noise is strong enough. Similar fast relaxation is also seen in Glauber Monte Carlo dynamics of the model, thus establishing the ubiquity of what has been reported earlier in particle dynamics (hence distinct from the spin dynamics considered here) of long-range interacting systems, that quasistationarity observed in deterministic dynamics is washed away by fluctuations induced through contact with the environment.

Ref. Debraj Das and Shamik Gupta, J. Stat. Mech.: Theory Exp. (2019) 084007

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Time : 4.50 pm - 5:05 pm

The dipolar spin glass transition in three dimensions

Tushar Kanti Bose [17]
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Dilute dipolar Ising magnets remain a notoriously hard problem to tackle both analytically and numerically because of long-ranged interactions between spins as well as rare region effects. We study a new type of anisotropic dilute dipolar Ising system in three dimensions [Phys. Rev. Lett. 114, 247207 (2015)] that arises as an effective description of randomly diluted classical spin ice, a prototypical spin liquid in the disorder-free limit, with a small fraction x of non-magnetic impurities. Metropolis algorithm within a parallel thermal tempering scheme fails to achieve equilibration for this problem already for small system sizes. Motivated by previous work [Phys. Rev. X 4, 041016 (2014)] on uniaxial random dipoles, we present an improved cluster Monte Carlo algorithm that is tailor-made for removing the equilibration bottlenecks created by clusters of effectively frozen spins. By performing large-scale simulations down to $x = 1/128$ and using finite size scaling, we show the existence of a finite-temperature spin glass transition and give strong evidence that the universality of the critical point is independent of x when it is small. In this $x \to 1$ limit, we also provide a first estimate of both the thermal exponent, $= 1.27(8)$, and the anomalous exponent, $= 0.228(35)$.

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