Recent Topics on Statistical Mechanics 2019

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Poster abstract book

Contents

Poster no. 1

Response of Glassy Liquids to Thermal Gradients

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We have studied the response of a model binary Lennard-Jones mixture [1], typical to manyamorphous alloys, to an externally applied thermal gradient, which is often encountered inmany real-life applications, using extensive non-equilibrium molecular dynamics simulations[2]. There is a flow of matter caused by temperature gradient, which is known as Soret effector thermophoresis. The interplay between the associated thermal diffusion and interdiffusionshow decoupling as the system approaches glass transition. Further, we also compute a phaseplot showing non-linear response for bigger gradients. By applying some heating-coolingprotocols, we show existence of long-lived non-stationary states.

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Poster no. 2

Effects of initial correlation on coarsening in uniaxialferromagnets: Scaling in growth and memory loss

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Theoretical studies of coarsening phenomena are concerned primarily about the sudden quenchof a completely spatially uncorrelated system to a point inside the ordered region. For a standardpara-to-ferromagnetic transition this corresponds to a rapid change of temperature from infinity to a value below the critical temperature T_c. Many experimental studies, however, have connections to shallow quenches. It is, thus, of substantial theoretical interest to learn how ordering progresses when initial configurations are prepared at finite temperatures, T_s, close to T_c. In this paper, we look at this broad picture of coarsening, via Monte Carlo simulations of ordering in uniaxial ferromagnets, starting with paramagnetic configurations having large equilibrium correlation lengths ξ. We address the question: does the growth rate of the average domain length,l , gets modified by the initial value of ξ? We observe, while the arrival of the scaling regime gets delayed with the increase of ξ, new equilibrium, for any finite system, is reached simultaneously, irrespective ofthe value of T_s. This implies, in the long time limit, for all $T_s > T_c$, systems grow not only with the same power-law exponent but also with the same amplitude. Evolution occurs in such a way as to forget the memory of correlated initial structure first, in a robust scaling manner. Completeloss of memory happens when l reaches ξ, beyond which growth data from different T_s collapse ontop of each other rather perfectly. From the merging lengths, thus, the static critical exponent ν can be quite accurately estimated.

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Poster no. 3

Dynamics and Structure of Self Propelled Particles

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The study of phase separation kinetics in active systems has been a topic of recent interest. Such active systems, which can be modelled using a collection of self-propelled Brownian particles with excluded volume interaction undergoes phase separation as a function of activity. Here we numerically study the phase behavior as well as the transport properties of this system as a function of interaction softness. We find that a change in the interaction softness can significantly alter the phase behavior as well as the structural properties.

Poster no. 4

Pattern formation in active furrowing

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Confined monolayers of motile bacteria such as Pseudomonas aeruginosa are known toproduce networks of furrows as they advance over soft agar substrates. The morphologyand overall expansion rates of such colonies appear to depend on the mechanical propertiesof the substrate. To understand this behaviour, we propose a minimal model of self-propelled rods furrowing through a passive medium consisting of particles that offerelastic resistance to being displaced from their equilibrium positions. Active particles at theadvancing edge of a colony create furrows that subsequent cells follow. We investigate the conditions under trail-following behaviour (stigmergy) emerges and the influence of dimensionless model parameters on the morphology of the furrows initiated at the edge and the subsequent evolution of the furrow network. Our results explain the physical origins of furrow networks in bacterial colonies

Poster no. 5

Morphological transitions of active Brownian particle aggregates on porous walls

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Active Brownian Particles (ABP) are well known to form motility induced aggregates at sufficiently large propulsion velocity and density. In the presence of a rigid wall, ABP's preferentially aggregate on the wall at low density. Here, we numerically study the aggregation of such particles on a porous wall which allows the particles to cross. We show that for a range of poresizes, the cross-wall particle flux is a non-monotonous function of particle velocity. Further, we show that for high wall porosity, the structure of the aggregate prefers multiple, disconnected clusters over a single, continuous, connected cluster, showing bistable behavior in cluster geometry for certain parametric regimes. The probability of having disconnected clusters is found to increase with activity. By calculating mechanical properties like pressure and surface tension, as has been introduced recently in active systems, and by using arguments from wetting theory, we try to justify why there is less spreading in this parameter regime.

Poster no. 6

A comparative study of dynamics of supercooled Kob-Anderson Binary Mixture and linear FENE polymers with their Week-Chandler-Anderson models.

Keshav Thakur, Duni Chand Thakur and Prasanth P Jose

The interplay between attractive and repulsive interaction governs the dynamics and structure of liquid. The Week-Chandler-Anderson (WCA) model shows that at higher densities the structure of liquid mostly depends on repulsive interaction. Recent studies on the WCA model of the glassforming KA binary mixture at high density supercooled state shows that even at high densities and at low temperatures the dynamics of binary mixture and its WCA (KAWCA) model show difference in the relaxation dynamics of the system; only at very high densities their dynamics approaches each other. We argues based on the mean force field that in Kob-Anderson mixture the small size of the A-B interaction is responsible for this observed behavior. In KA binary mixture the glass formation in induced due to frustration induced by the B particles. In order to further test difference in thedynamics we have compared the difference in dynamics of a linear polymer model where Lennarnd-Jones beads are connected by springs where frustration is due to bonding interaction between thebeads. In this model all particles are of identical size thus the equivalent dynamics observed inpolymer and its WCA model at much lower density as compared to KA model and its KAWCA. Thus our analysis show that the observed difference in the dynamics in the KA binary mixture is dueto presence pf smaller size of the B particles in the KA binary mixture.

Poster no. 7

Grand Canonical ensemble formulation of quartic oscillators

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Thermodynamic quantities like entropy, average energy and specific heat have been derived in microcanonical and canonical Ensemble[1,2] for quartic oscillator. From the results, it is found that Statistical Mechanics of finite dimensional systems is a very good method for the description of the developed chaos in small dimensional Hamiltonian systems. In this paper we obtain the thermodynamics of N dimensional quartic oscillators in Grand Canonical Ensemble (GCE).

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Poster no. 8

Velocity Auto-Correlation of a confined Brownian particle

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Motivated by the dynamics of an active particle, we studied thestochastic dynamics of a Brownian particle in the presence of a linear velocity depen-dent force $f_s(1\frac{v}{v_s})$, where f_s is constant. We have exactly calculated the velocity auto correlation function(VAF)in different situations of the dynamics. We observe that the VAF decays exponentially with time and saturates to a constant value in the time assymptotic limit for a fixed f_s. Increase of f_s value slowly destroys the correlation in velocities at different times. As a result VAF saturates faster with f_s values. Further in the presence of a sinusoidal driving force, the VAF gets suppressed with the amplitude of driving.

Poster no. 9

A totally asymmetric simple exclusion process with quenched hopping rates and periodic boundaries

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Totally asymmetric simple exclusion process (TASEP) is a non equilibrium model which mimics various biological transport phenomena like RNA translation by ribosome[1,2], ribosome translocation along mRNA loops[2,3]and physical transport phenomena like vehicular transport in closed network[4], etc. Among various other methods,Mean field theory[5]is the simplest approach to study the steady state in a TASEP. Introduction of interactions leads to change in dynamics. Following scenario provides an intuitive picture to introduce interactions in the system; in case of vehicular traffic, the speed of car not only depends on speed restrictions but also on its distance from the car ahead of it.It is observed that in a closed TASEP with quenched hopping rates, Mean Field theory fails as soon as the interactions are introduced in the system. So, Cluster Mean Field theory is deployed to study the steady state andMonte Carlo simulation is applied to confirm the results.

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Poster no. 10

Efficient search and capture via dynamic microtubules orchestrate centrosome relocation during IS formation

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Upon contact with antigen presenting cells (APCs) cytotoxic T lymphocytes (T cells) establish a highly organized contact zone denoted as immunological synapse (IS). The formation of the IS impliesrelocation of the microtubule organizing center (MTOC) towards the contact zone, a process necessary to kill the APCs by subsequent secretion of cytotoxic material at the IS via exocytosis. Mechanically the centrosome repositioning is driven by dynein via a MT end-on capture-shrinkage operating at the center of the IS [1]: a subset of MTs is captured by dynein anchored at the IS cortex. The dynein power stroke then reels in the captured MTs, which depolymerize (shrink) when pulled against the IS cortex. The effectiveness of the capture-shrinkage mechanism depends on how efficiently the MTs while being anchored at the MTOC, find the IS and thereby bound with the cortically anchored dynein at the IS center. To explore the effectiveness of this process, we propose a stochastic search and capture model that assumes astral MTs grow and shrink rapidly in all directions from the MTOC, probing the inner surface of the plasma membrane until they capture a small dynein patch at the center of theIS. In this study, we develop simple mathematical and numerical models incorporating relevant components of a cell and propose an optimal search strategy.

Poster no. 11

Asymptotic velocity distribution of a one dimensional driven binary granular gas

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A central question in the theory of driven granular gases is the nature of the tails of the velocity distributions. In driven binary systems, experiments have reported different velocity distributions for the different components. The typical experiment consists of two layers: the bottom layer is driven externally while the top layer is excited by the bottom layer. The two distributions are found to be asymptotically $e^{-v^{3/2}}$ and e^{-v^2} for the bottom and the top layer respectively. Here, we consider a mixture consisting of two types of particles and the external driving acts only on oneof the components. We assume the well mixed limit and that the rate of collision is independent of relative velocity. The change in velocities v' due to driving is given by $v' = r_w v + \eta$ where $r_w \in [1, 1)$ and η is the noise taken from a fixed distribution. This form allows us to realisedifferent cases of driving depending on the parameter r_w. We show that the variance and the two particle velocity correlation functions form a closed set of equations. In the thermodynamiclimit, the velocity correlations vanish and we derive an exact formula for the variance of the two types of particles. Higher order moments of the velocity distribution depend on moments of lower order. The tail of the steady state velocity distributions is obtained by analysing the ratios of large moments. We show that the tails of the velocity distribution for both types of particles have identical behaviour, even though they are driven differently. We show that the tail of the steady state velocity distribution is non-universal and depends on the nature of the driving for $r_w < 1$ whereas for diffusive driving ($r_w = 1$), the velocity distribution is universal.

Poster no. 12

Flow can order: Ordered states of live XY spins in two dimensions

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We present the hydrodynamic theory of active XY spins coupled with flow fields, both with andwithout number conservation in two dimensions (2D). For the number non-conserving case with livespins, the system can synchronize, or be phase-ordered for sufficiently strong flow-phase couplings with various types of order, e.g., quasi long range order (QLRO) or new kinds of order weaker orstronger than QLRO. For the number conserving case, the system can show QLRO or order weaker than QLRO, again for sufficiently strong flow-phase couplings. We calculate the variance Δ of phase fluctutions, which scales with the logarithm of system size(L) as $\Delta \sim (\log L)^{\mu}$ with different values of μ corresponding to different kinds of order. For other choices of the model parameters, the system necessarily disorders in a manner similar to immobile but active XY spins, or 2D Kardar-Parisi-Zhang surfaces.

Poster no. 13

An in silico approach for centrosome separation during prophase

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Proper centrosomal separation during prophase of mammalian mitosis is crucial for identical segregation of the DNA. Mechanical activities of the molecular players coordinating this separation remains unclear due to elusive role of Kinesin-5, a plus end directed molecular motor that can slideanti-parallel microtubules. Interactions of the centrosomal microtubules with cellular objects (e.g.cortex, cell wall and nucleus) generate forces on the centrosome, thereby promotes centrosomal movements. Using an in silico model, we show that a combined interaction of microtubule withcortex, cell-membrane and nucleus can fully separate the centrosomes.

Poster no. 14

CONFINED FILAMENTS IN SOFT VESICLES - CASE OF SICKLE RED BLOOD CELLS

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Abnormal shapes of red blood cell (RBC) cause various diseases. RBC morphology is also important for learning physics of bio-membranes. Here we focus on sickle shaped RBC which form due to abnormal growth of semi-rigid Hemoglobin (HbS) fibers confined in RBC. Using the standard area difference elasticity (ADE) model for RBC and worm-like chain model for the confined HbS fibers, we study shape deformations at equilibrium using Monte-Carlo simulation. We show while a single HbSfiber is not rigid enough to produce sickle-like deformation, a fiber bundle can do so. We also consider multiple disjoint filaments and find that confinement can generate multipolar RBC shapes and can even promote helical filament conformations which have not been discussed before. The same ADE model,in different parameter regime, appropriate for microtubules confined in phospholipid vesicles, can giverise to tubulation. We also reproduce tube collapse transition and tenis racket type shapes, as seen in experiments. We conclude that with a decrease in the surface area to volume ratio, and membrane rigidity, the vesicle prefers tubulation over sickling. We reproduce various non-axisymmetric vesicleshapes, which have been observed experimentally, both in the context of sickle RBC and phospholipid vesicles, but have not been addressed by theoretical models yet.

Poster no. 15

Dynamics of tagged particles in a biased $A + A \longrightarrow \emptyset$ system in one dimension

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Dynamical features of tagged particles are studied in one dimensional $A + A \longrightarrow \emptyset$ system on a periodic lattice,where the particles A have a bias ($0 \leq \epsilon \leq 0.5$) to hop one step in the direction of their nearest neighboring particle. $\epsilon = 0$ implies purely diffusive motion and $\epsilon = 0.5$ represents purely deterministic motion of the particles.Initiallythe lattice sites are filled with particles (sayA) with some probability. At each update a site is selected randomly and if there is a particle on it, it moves towards its nearest neighbor with probability ϵ and otherwise in the opposite direction. If there is already another particle located on this neighbouring site, then both particles are annihilated. We show that for $\epsilon > 0$, probability distribution of the particles P(x, t) shows a double peak structure with a dip at x= 0 and at late time regime it assumes a double delta functional form. For any ϵ, there is a time scale t which demarcates the dynamics of the particles. Below t, the dynamics are governed by the annihilation of the particles,and the particle motions are highly correlated, while for $t \gg t^*$, the particles move as independent biased walkers. t^* diverges as $(\epsilon - \epsilon_c)^{-\gamma}$ where $\gamma = 1$ and $\epsilon_c = 0.5$. ϵ_c is a critical point of the dynamics. At ϵ_c, the probability S(t),that a walker changes its direction of motion at timet, decays as $S(t) \sim t^{-1}$ and the distribution $D(\tau)$ of the time interval τ between consecutive changes in the direction of a typical walker decays with a power law as $D(\tau) \approx \tau^{-2}$.

Poster no. 16

Thermodynamic uncertainty relation in thermal transport

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We use the fundamental nonequilibrium steady state fluctuation symmetry and derive a condition on the validity of the thermodynamic uncertainty relation (TUR) in thermal transport problems, classical or quantum alike. We test this conditionand study the breakdown of the TUR in different thermal transport junctions of bosonic and electronic degrees of freedom. First, we prove that the TUR is valid in harmonic oscillator junctions. In contrast, in the nonequilibrium spin-boson model,which realizes many-body effects, it is satisfied in the Markovian limit, but violations arise as we tune (reduce) the cutoff frequency of the thermal baths, thus observing non-Markovian dynamics. Finally, we consider heat transport by noninteracting electrons in a tight-binding chain model. Here we show that the TUR is feasibly violated by tuning e.g. the hybridization energy of the chain to the metal leads. These results manifest that the validity of the TUR relies on the statistics of the participating carriers, their interaction, and the nature of their couplings to the macroscopic contacts (metal electrodes, phonon baths).

Poster no. 17

Polar flock with bond disorder

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Understanding the collective behaviour of self-propelled particles isan active area of research. In most of the natural system we always observe only one type of species moving together. Although different species differ in their biological complexity and interaction ability, but thay are common in one sense that thay are all active and have tendency to interact with their neighbours. In our model we have introduced a random distribution of interaction strength parameter to all the particles. Strength of interaction for each particle is quenched in time. When all the particles have same interaction strength, the model reduces to famous Vicsek model (Vicsek et al. Phys. Rev. Lett. 75, 1226 (1995)). We ask the question, what is the steady state of the system for different interection strength? Starting from random homogeneous state how the system evolve towards an ordered/clustered state?

Poster no. 18

Ordering kinetics of passive particles in active medium

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Understanding the phase ordering kinetics in an active system is an interesting area of research. There exist many anomalies that are observed near the critical point in static and dynamic properties. Phase ordering kinetics involves evo-lution of order parameter that consists conserved and non conserved kinetics depending upon the conserved or non-conserved nature of fields. The system with nonconserved kinetics (i.e model A) and the system involving conserved kinetics (i.e model B) are the systems which are well studied. Recently few studies are done on conserved active model, or active model B. But not much is explored for kinetics of conserved passive model in the presence of active particles. In our study we focus on the study of ordering kinetics of passive particles in the presence of active particles.

Poster no. 19

Availability versus storage capacity: Phases of asymmetric exclusion processes competing for finite pools of resources

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We address how the interplay between the finite availability and storage capacity of particles at different parts of a spatially extended system can control the steady state currents and density profiles in the quasi one-dimensional current-carrying channels connecting the different parts ofthe system. Setting it up as a minimal model consisting of two particle reservoirs of finite storage capacity connected by two anti-parallel asymmetric exclusion processes (TASEP) of equal size, westudy the steady state currents and densities in the two TASEP lanes. The ensuing phases andthe phase diagram are parametrized by the model parameters defining particle exchange between the TASEP lanes and the reservoirs, and the filling fraction of the particles that determine the total resources available. Being controlled by these parameters, the two TASEP lanes can be foundin the same or different phases, including a pair of delocalized domain walls, or a single localized domain wall and a spatially constant density.

Poster no. 20

Flocking transition in the q-state active Potts model

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We consider the Active q-state Potts model (APM) with q = 4 in two-dimensions. The active particles can change their internal states and also undergo a nearest neighbor biased diffusion which results a flocking model. The flocking dynamics is exploited to probe the liquid-gas phase transition in the APM with an intermediate liquid-gas co-existence phase. We compute the phase diagram for the APM and analyze the effect of self-propulsion velocity on the particle arrangements in the co-existence phase. We further construct a coarse-grained hydrodynamic descriptions of the model which validates the findings of microscopic simulations.

Poster no. 21

Analyses of Interactive TASEP with Dynamic Defect: Theory and Simulations

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Biological molecular motorsarethe special enzymes that play a vital role in RNA translation by ribosomes, intracellular transport, transport in ion channels and many other cellular processes. The motor proteins carry cellular cargo and move in one preferred direction triggered by the conversion of chemical energyto mechanical energy.These transportation mechanisms are characterized under the category of non-equilibrium class. The model that encrypts the functional module of motor proteins is totally asymmetric simple exclusion process (TASEP) where the dynamics is driven by constant supply and dissipation of energy. The microtubules are considered to be a one-dimensional lattice with motor proteins as point particles. The prototype to study the dynamics of motors is made more realistic by considering particle-particle interactions. Moreover, the motion is not always smooth, infact, some molecular motors act as defect that serves as a hurdle to moving particles. The switch on/off kinetics of defects gives an additional variant of TASEP model. Motivated by the biological scenarios, an interactive model is studied with a dynamic defect.A theoretical approach is developed that analyses thedynamic properties of model with various parameters that governs the system. The results are tested with Monte Carlo simulations.

Poster no. 22

Migration of DNA chain confined under a solvent gradient

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We consider a double stranded DNA (dsDNA) confined between two walls of a strip of finite width. We investigate the effect of solvent gradient on the transfer of dsDNA from one wall to the other. For this amutually self-attracting self-avoiding walk model of polymer have been considered on the square lattice. The base-pair intercations between the two starnds across the strip have been varied to model the solvent gradient. Using the exact enumeration technique we explored the effect of sequence and solvent gradient on the melting profile of DNA. The simple model presented here captures essential physics of transport process such as DNA thermophoresis.

Poster no. 23

Tumbling dynamics of a dumbbell in viscoelastic shear flow

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We study harmonically coupled particles in a viscoelastic shear flow. Using analytical calculations we show that the center of mass diffuses as $x_c^2(t) \sim t^\alpha + 2$, where $0 < \alpha < 1$ is the exponent of subiffusion, generalizing the results of McPhie and co-workers, Physica A299, 412 (2001). The motion of the relative coordinate is quite intriguing, in that $x_r^2(t) \sim t^{2(1-\alpha)}$, and exhibits all three kinds of motion- subdiffusive, normal diffusion and superdiffusive. This implies nonexistence of a steady state, in sharp contrast with the known results for motion in purely viscous flows. We discuss reasons for these differences.

Poster no. 24

Steady state analysis of a two-channel exclusion process with dynamic disorder

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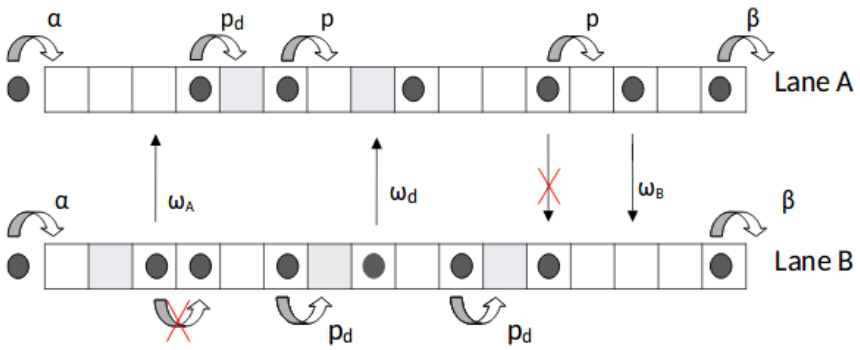
During transcription of genes, a molecular motor - the RNA polymerase - attaches itself to a specific promoter region of DNA (transcription start site), read off the DNA sequence adding RNA nucleotides to create messenger-RNA(mRNA) sequence and escapes from DNA(transcription endsite). The translation involves decoding of mRNA in a ribosome to produce amino acid chain. The free diffusing transfer-RNA(tRNA) binds to specific mRNA codon and carry the amino acidchain. Protein expression can be regulated by exploiting the relative concentrations of tRNA incytoplasm that determines ribosome translation rate. The DNA-bound proteins acts as disorder in the pathway of RNA polymerase and slows it down which may cause neuro-degenerative diseases. The disordered process can be modeled using discrete lattice gas model TASEP(Totally asymmetric simple exclusion process) with site-wise disorder in a two-channel system(shown in Fig. 1). The particles representing molecular motors in a cell are distributed randomly obeying hard-core exclusion principle which states that not more than one particle can occupy same site on the lattice. The unconstrained defect dynamics are considered in which a defect can bind/unbind dynamically to any site irrespective of particle occupancy. The rate of forward hopping(p_d) in the presence of defect is slower than the normal particle hopping rate(p). The continuum mean-field equations of the model are derived and then solved numerically to obtain steady-state phase diagrams. The role of various parameters namely defect (un-)binding constants, lane-changing rateshas been thoroughly examined. The defect (un-)binding rates are found to affect the phase bound-aries in phase plane. The effect of system size on the steady-state dynamics of the system has also been analyzed. The extensive Monte Carlo simulations yields good estimation with mean-field results.



(a)

Figure 1: (a) Schematic diagram of a coupled two-channel TASEP with dynamic disorder. α and β are the entrance and exit rates respectively. The defect is represented as shaded site. Crossed arrows indicate forbidden transitions.

Poster no. 25

Dynamics of binary colloids in the influence of external potenial

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The molecular dynamics simulations of a binary colloidal mixture of soft spheres, subjected to an external repulsive potential, reveal that the attractive depletion interaction between the barrier and larger particles alters the dynamics of the system significantly at lower tempertaures. The larger particles diffuse faster than the smaller particles over the potential barrier and the smaller particles get localized in between the potential barriers at lower temperatures, mimicing a dynamics similar to system undergoing a glass transition. The anomaly in self diffusion coefficients of both the species reveal that the diffusive dynamics of the larger particles exhibit sub-Arrhenius temperature dependence at low temperatures, in contrast to the beleif of its quantum tunnel origin. The activation energy of the larger particles is found to be temperature dependent and hence changes the effective barrier height accordingly; while that of smaller particles is temperature independent. The waiting time distributions and free energy of interactions of both the species of particles verify the nature of the dynamical properties of the system. However the dynamics approach towards classical regime, i.e, the larger particles show super-Arrhenius diffusion, as the density of the particles increases. Similaraly, in the influence of asymmetric external potential, the dynamics of larger particles show a transition from sub-Arrhenius to super arrhenius behaviour with the increase in the asymmetry of the external potential at low temperatures and density.

Poster no. 26

Study of the tricritical Ising universality class using conformal bootstrap in two to three dimensions.

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Conformal field theory is a quantum field theory with conformal symmetry. We use the conformal bootstrap technique which consists of conformal invariance and crossing symmetry. Using this technique, we have studied the tricritical Ising universality class in two to three dimensions. By studying bootstrap constraints originating from multiple correlators on the CFT data of multiple OPEs, we are able to determine the scaling dimension of the spin field Δ_σ in various non-integer dimensions $2 < d < 3$. Δ_σ is connected to the critical exponent η that governs the (tri-)critical behavior of the two-point function via the relation, $\eta = 2d + 2\Delta_\sigma$. Our results for Δ_σ match with the exactly known values in two and three dimensions and are a conjecture for non-integer dimensions. We also compare our CFT results for Δ_σ with ϵ-expansion results, available up to ϵ^3 order. Our techniques can be naturally extended to study higher-order multi-critical points.

Poster no. 27

Emergence of a bicritical end point in the random crystal field Blume-Capel model

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Blume Capel model is a spin model that describe the phenomenology of a variety of physical systems, such as liquid mixtures of $^3He -^4 He$, metamagnets, alloys of magnetic and non magnetic materials, ferroelectrics, liquid crystals and others. It has a rich phase diagram which consists of three critical lines meeting a first order line at a tricritical point. We obtain the phase diagram for the Blume-Capel model with bimodal distribution for random crystal fields, in the space of three fields : temperature (T), crystal field (Δ) and magnetic field (H). We find that the topology of the phase diagram changes as the strength of the disorder increases. Three critical lines meet at a tricritical point for weak disorder. As disorder strength increases there is no tricritical point in the phase diagram. We instead find a bicritical end point, where only two of the critical lines meet on a first order surface in the H = 0 plane. For intermediate strengths of disorder, the phase diagram has critical end points (where a second order transition line terminates at a first order line) along with the bicritical end point.

Poster no. 28

Re-entrant phase separation in nematically aligning active polar particles

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We present a numerical study of the phase behavior of repulsively interacting active polar particles that align their active velocities nematically [1]. The amplitude of the active velocity, and the noise in its orientational alignment control the active nature of the system. At high values of orientational noise, the structural fluid undergoes a continuous nematic-isotropic transition in active orientation. This transition is well separated from an active phase separation, characterized by the formation of high density hexatic clusters, observed at lower noise strengths. With increasing activity, the system undergoes a re-entrant fluid- phase separation- fluid transition. The phase coexistence at low activity can be understood in terms of motility induced phase separation. In contrast, the re-melting of hexatic clusters, and the collective motion at low orientational noise are dominated by flocking behavior. At high activity, sliding and jamming of polar sub-clusters, formation of grain boundaries, lane formation, and subsequent fragmentation of the polar patches mediate remelting.

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[1] Soft Matter, 2019, DOI: 10.1039/C9SM00998A

Poster no. 29

Casimir Effect and Smearing Thermal Field

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The Casimir effect [1] accounts for an interaction between two metal plates.This was calculated by measuring the change in thermodynamic electromagnetic zero-point energy by changing the distance between the plates. It was interpreted that the electromagnetic fluctuations whose wavelength is comparable with the distance between the plates would be contributing to the Casimir effect, and the interaction is independent of the material of theplates. This result is universal depending only on h,c and the distance between the plates in the limit of absolute zero temperature. Lifshitz [2] and Schwinger et al. [3] used their own formalism to expand the field theory for higher temperatures. However, it is obvious from the discussion by Breviket al. [4] that the temperature dependence on the Casimir effect is not completely understood. Traditionally, Casimir effect is derived from quantum field theory perspectiveby quantizing the thermal field to calculate the energy of the ground state zero-point fluctuations. Landau-Ginzburg field theory is usually applied to systems for understanding phase transitions. Instead, here we use it to analyze thermal field in the limit of absolute zero temperature and study the fluctuations in such field. We qualitatively attempt to study the thermal field as a statistical field and consider correlation length of the thermal field fluctuations comparable with distance between the plates in Casimir effect.

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Poster no. 30

Escape From Morse Potential Driven ByGaussian White Noise

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We study the dynamics of a Brownian particle in Morse potential under thermal fluctuations, modeled by Gaussian white noise with amplitude playing the role of absolute temperature. Dynamics of such a particle is investigated by numerically integrating the corresponding Langevin equa-tion. From the average first passage time (escape time), we study the temperature dependence of Kramers reaction rate using vant Hoff-Arrheniusplot. For additive noise, it is observed that the reaction rate increases monotonically with temperature. Further, nonlinearity in the plot also suggests that temperature dependence of reaction rate does not follow Arrhenius equation, which is usually valid for non-interacting (ideal) system. In comparison to additive noise, we demonstrate that escape time is shorter for multiplicative noise, implying that reaction is accelerated in the latter form of fluctuations.

Poster no. 31

A chemical kinetic basis for measuring translation initiation and elongation rates from ribosome profiling data

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Analysis methods based on simulations and optimization have been previously developed to estimate relative translation rates from next-generation sequencing data. Translation involves molecules and chemical reactions, hence bioinformatics methods consistent with the laws of chemistry and physics are more likely to produce accurate results. We derive simple equations based on chemical kinetic principles to measure the translation-initiation and individual codon translation rates from ribosome profiling experiments. Our methods reproduce the known rates from ribosome profiles generated from detailed simulations of translation. By applying our methods to data from S.cerevisiae cells, we find that the extracted rates reproduce expected correlations with various molecular properties. Our analysis further reveals that a codon can exhibit up to 26-fold variability in its translation rate depending upon its context within a transcript. This broad distribution means that the average translation rate of a codon is not representative of the rate at which most instances of that codon are translated, and it suggests that translational regulation might be used by cells to a greater degree than previously thought.

Poster no. 32

Totally Asymmetric Simple Exclusion Process with Interacting Particles on Network Junctions

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Biological transport phenomena frequently exhibit complex network behaviour when several molecular motors converge to special junctions. Moreover,several other motors move out from these junctions in different directions.Recent experimental observations suggest the presence of nearest neighbour particle interactions. Stimulated by these observations, we developed a theoretical framework to investigate network junction models of totally asymmetric simple exclusion processes with interacting particles. We employed the two cluster mean-field approach, which takes into account short range correlations in the system. Using the approach, we explicitly computed the phase diagrams, density profiles and correlation profiles and found that their existence is dependent on the total number of outgoing, incoming segments and the interaction energy among the particles. It is observed that the correlations weaken in a network with a greater number of incoming or outgoing segments. All theoretical results are in good agreement with extensively performed Monte Carlo computer simulations.

Poster no. 33

Collective excitations of two-dimensional Bose-Einstein condensate inliquid phase

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Liquid formation of the dilute ultracold atomic system is one of the most exciting topics in Bose-Einstein condensate (BEC). The droplets have been observed in the isotropic short-range interacting system of two species of cold atoms as well as in the anisotropic long-range dipolar interacting system of 164^{Dy} or 166^{Er} atoms. In the mixture of two components Bose atoms, the spherical droplet has been observed under the competition between the effective short range attractive interaction and the repulsive interaction due to the quantum fluctuation. The two component BEC may be the mixture of atoms of two different elements (different atomic mass) or maybe the mixture of atoms with two different internal degrees of freedom of a given element.

Three-body collisions limit the lifetime of the droplets. In the lower dimensions, it is expected that this lifetime can be extended because of reduced phase-space available to colliding atoms. That is why people have an interest in droplets in the lower dimension. BEC can be deeply affected by spin-orbit coupling (SOC), induced by theapplication of two laser beams. We have studied the ground state properties of the two dimensional BEC of atoms with different types of SOC such as Rashba, Dresselhaus and Raman SOC. To understand the exact nature of the correlated system, the study of collective excitation is very important and necessary. We have calculated the collective excitations of this system using Bogoliubov theory. We find that the spectra contain single or double rotons depending on the various interaction strength.

Poster no. 34

Temporal cooperativity in a group of elastically coupled motor proteins in a harmonic trap

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Motor proteins are organic macromolecules found in eukaryotic cells, each with a unique structure and function. Motor proteins perform numerous functions like muscle contraction and transportation of intracellular cargoes. The outcome of multiple motor-driven intracellular transport processes depend crucially on their collective behavior. In particular, tug-of-wars between groups of antagonistic motor proteins (e.g. kinesin and dynein), where both teams bind simultaneously to a cargo and thereby stall each other, has attracted a lot of attention. The result of a tug-of-war is dictated by the collective stall time of a motor team; a team with larger stall time is more likely to win. In a recent paper (B.S and M.G, Phys. Biol. 16, 016006, 2019), we studied how the the stall time T_N depends on the totalnumber N of motors, assuming equal sharing of opposing load between all motors. We showed that a generic motor may behave cooperatively (stall time increasing with N), or non-cooperatively, depending on its biophysical properties. Here, we investigate cooperative behavior in a more realistic model of a motor-cargo assembly. We simulate a one-dimensional stochastic model, where each motor is linked to the cargo through an elastic spring with stiffness constant . In this model, each motor performs forward and backward hopping motions on the filament, the rates for which are different because of the free energy change associated with ATP hydrolysis. Apart from forwardand backward hopping, motor bind to, and unbind from, the filament with specific rates. The bead is subjected toelastic force originating from the stretched motor-springs, thermal noise as well as an external force from an opticaltrap with a specific trap stiffness $_t$,. We constructed a Gillespie code which can simulate up to six motors. Somerepresentative results from our simulations with kinesin-1 motors are shown below in Fig. 1 and 2. Our resultsindicate that emergence of cooperative behavior is closely connected with the load-sharing properties of the team.

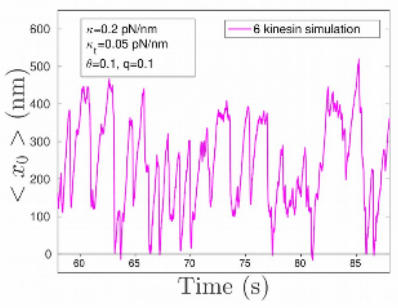

Fig.1

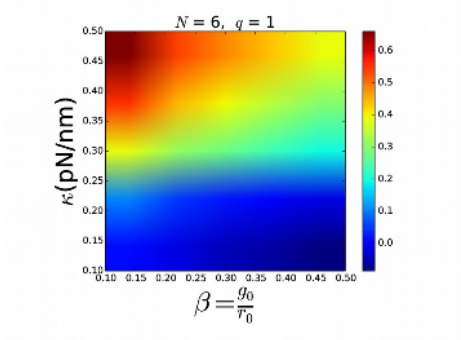

Fig.2

Fig.1: Time traces of average cargo position(<x_0>) in the presence of trap with trap stiffness K_t=0.1pN/nm and motor linker stiffness K=0.1pN/nm. The total number of motors on the bead is N=6.

Fig.2: A colour-coded "phase diagram" for kinesin like motors in the β-K plane by taking ln T_N(K,β) /N as the order parameter. Here, β is the ratio of intrinsic detachment and attachment rates of a single motor.

Poster no. 35

Unequal load-sharing in force-induced catastrophes for a microtubule bundle

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Microtubule filaments are important components of the cytoskeleton of a eukaryotic cell, which play important roles in various vital processes such as intracellular transport, chromosome segregation and cellmotility. Microtubules are polymeric filaments, whose basic building unit is a hetero-dimer of alpha andbeta-tubulin proteins. Various experimental studies have revealed many interesting aspects about the unique dynamical properties of microtubules. In particular, the spontaneous and abrupt transition of a growing microtubule to a shrinking one, called catastrophe, has been the subject of a large number of mathematical, computational and experimental studies. It is now well-established that a catastrophe event is triggered bythe hydrolysis of GTP in beta-tubulin, and the consequent loss of structural stability. In intracellular environment, growth of microtubules is often hindered by the presence of barriers of various kind, such askinetochore complexes and cell cortex, which impact their polymerisation force and dynamical properties such as catastrophe frequency. Here, we study the effect of a forced barrier on the statistics of catastrophe events in a single microtubule as well as bundle of two microtubules. We use a one-dimensional stochastic model of a microtubule with random growth and hydrolysis, interacting with a rigid barrier which is subjected to thermal noise and an external force. Our mathematical results predict that the catastrophe frequency of a single filament monotonically increases with the force and saturates at large forces, in agreement with Monte Carlo simulations (Fig.1). The study is extended to a bundle of N filaments; here,while a mean-field extension of the theory predicts equal sharing of the total applied load between the filaments, numerical simulations for N=2 suggest a very uneven distribution of the load. The deviation from the mean-field prediction is characterized using a dimensionless load-sharing parameter.

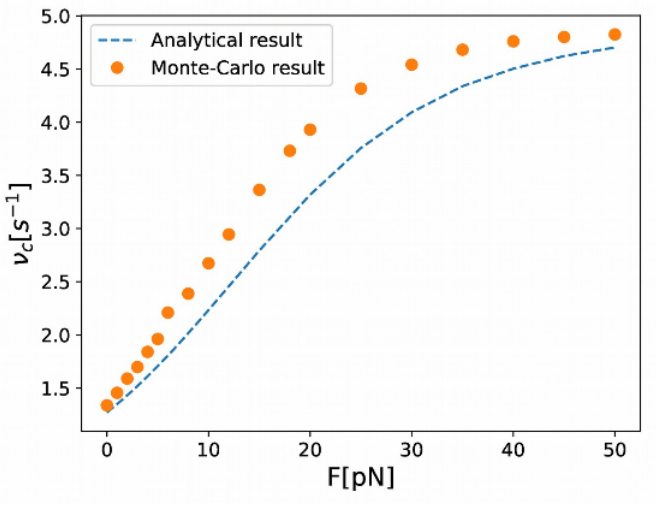

Fig.1: *Comparison of the theoretical prediction and numerical results for a single filament growing against a forced barrier.*

Poster no. 36

Pressure Induced Phase Transitions in Liquid Crystals - A Molecular Field Approach

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Study of phase transitions in liquid crystalline materials are of very much importance due to their wide and various applications. Different experiments had been successfully done to show the existence of different liquid crystalline phases. Although the mean field theory of nematic liquid crystals by Maier and Saupe [1] in 1960, can correctly predict the existence of a first order phase transition between the nematic and isotropic liquid states, no pressure dependence can be investigated using this formula. In 1980, Luckhurst and Romano [2] had taken an anisotropic part of the potential along with the isotropic part and used this potential to computer simulation to find the phase diagram for some liquid crystals. But they had not done any pressure variation. Also a rigorous microscopic treatment of a nematic fluid system based on a pairwise interaction potential is immensely complex. For studying pressure dependence of such systems mean field theories are often the standard method of choice. In this paper [3] we have chosen a simple effective potential

$$U = u^4/v^4 - u_2/v^2 - Au_2/v^2 < P2 > P2(cos\theta))$$

to study an isothermal-isobaric (NPT) ensemble describing a liquid crystalline system. Using this we have studied in particular the pressure dependence of liquid crystalline phase transitions. where, u_2, u_4 and A are constants, v is the mean molecular volume, θ is the angle between the director and the molecular long axis, $< P2 >$ is the nematic order parameter.

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Poster no. 37

Cosmological phase transitions in an expanding universe

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Cosmological phase transition has emerged as a new phenomenon in the gravitational clustering of galaxies. We make use of statistical mechanics and thermodynamics to develop the partition function for an ensemble of galaxies. From the partition function, entropy changes are calculated and are studied with the correlation energy. The entropy graphs show an interesting phenomena where the idea of low clustering to mild clustering and then to high clustering exhibit the phenomena of phase transitions. These phase transitions are entirely different from the phase transitions in materials science. Here the symmetry breaking idea gets explored very interestingly. We also discuss quantities like latent heat and explanation of these quantities from thermodynamic point of view add considerable knowledge for explaining the phenomena of cosmological phase transitions.

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Poster no. 38

Microscopic structure of confined binary fluid mixture at demixing transition

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Phase transitions are well understood in bulk systems, but there are instances where the confinement makes an essential difference [1]. Inspite of the rich phenomenology, there have been theoretically few investigations [2,3], though there continue to be many experimental studies [4]. Here, we investigate the phase separation behaviour near the consolute point of thin symmetric binary fluid films (AB) confined between neutral, asymmetric and symmetric parallel walls using molecular dynamics simulations. The pairwise interactions between the particles are modeled by the Lennard-Jones potential, with parameters that lead to demixing transition in the bulk. For neutral walls, where there is no preferential attraction of any of the components towards the wall, we find that the phase separation occurs at low temperatures as compared to its bulk counterpart. The estimation of the critical temperature is carried out by the intersection criterion of the Binder cumulant using subsystem analysis method. The critical exponents for the correlation length and the concentration susceptibility has also been determined from the time avearged static structure factor. In symmetric confinement, we find that A-rich surface enrichment layers form quickly during the early stages of the evolution causing a depletion of A in the inner regions of the film. These surface-directed concentration profiles propagate from the walls towards the center of the film, resulting in a transient layered structure. These structural heterogeneities are tracked as a function of the distance from the confining wall. In asymmetric confinement when both the walls prefer the different components of the binary mixture, we find that the densities are essentially not conserved in the thin film of binary fluid, and hence the behavior differs strongly from spinodal decomposition in the bulk.

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Poster no. 39

Condensation of Hard sphere Bosons using cluster expansion

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The phenomenon of Bose Einstein condensation in hard sphere Bose gas is explained using the modified Mayers cluster expansion method by Ushcats. The saturation density is found out from the values of irreducible cluster integrals calculated with the help of s-wave scattering length.The result of saturation density is compared with the experimentally observed Bose Einstein condensate of Sodium-23 atomic vapor.

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Poster no. 40

Hysteresis in Random field Blume Capel model on Bethe lattice

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