Molecular dynamics investigation of the structural and dynamical response of polyampholyte chains to external magnetic field

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Many crucial phenomena set in due to the interaction between external fields and charges in softmatter systems. External magnetic field-dependent perturbations in these systems open avenues to many important technological applications. For in-stance, alignment of block copolymer domains [1], modifications of thermal conductivity of liquid crystal networks [2], etc. Theoretical study of 2d plasma in a magnetic field shows that the static properties are unaffected by the field. However, the mobility of the particles scales with the inverse of the magnetic field [3]. Despite experimental and computational research, a detailed understanding of the effect of external magnetic fields on polymeric materials is lacking. Here, we study a model semiflexible block polyampholyte chain in external magnetic fields using molecular dynamics simulation [4]. The magnetic vector potential is included in the kinetic part of the (modified) Hamiltonian of the system. We find that the radius of gyration and the persistence length decrease as the magnetic field increases. The induced magnetic moment of the chain enhances and aligns along the field direction. The in-plane diffusion of the chain center of mass perpendicular to the field decreases at the higher magnetic field. We observe that the effects are less pronounced for polyampholytes with random charge arrangements.

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pH dependent Hydration around Lysozyme protein

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Numerous experiments, such as X-ray scattering and neutron diffraction, show that solvent structure near biomolecules differs from bulk solvent. [1] This is supported by several theoretical studies. [2,3] Recent study using 2D IR spectroscopy and Molecular Dynamics (MD) simulation [4] examined pH-induced structural changes in Lysozyme, revealing significant effects of acidic side chain protonation on protein structure but not hydration dynamics. In our study, we use constant pH molecular dynamics (cpHMD) simulations to investigate the hydration water's static and dynamic properties around Hen egg-white Lysozyme (PDB ID 1AKI) at various pH levels. We focus on how pH affects the protonation of acidic residues and its influence on hydration. At acidic pH, the protein's overall charge is positive due to protonation of acidic residues, decreasing as pH rises and becoming negative at the isoelectric point. To study static properties, we calculate the radial distribution function (g(r)) of water around acidic residues under extreme acidic, neutral, and basic pH conditions. The rdf value is lower at acidic pH due to reduced electrostatic interactions. For dynamics, we calculate the self-diffusion coefficient of hydration water from the long-time behavior of MSD, finding higher diffusion at low pH, with a sharp decrease near the isoelectric point due to charge inversion. Our findings highlight how pH dependent protonation of acidic residues significantly impacts the hydration water's static and dynamic properties.

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Cohesion of walls mediated by polymer melts

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The behavior of confined polymer melts in shear flow lies in their relevance to practical applications like lubrication and transport properties[1].We have studied confined polymer melt under Shear. In this study, we use Nonequilibrium Molecular Dynamics (NEMD) simulation to understand different rheological properties and adhesion of walls in presence of polymer melt. We find that the density profiles for monomers and solvents are insensitive to shear rate[2]. Under shear, the chains have a tendency to reorient in the flow direction. For all different wall-solvent, wall-polymer and polymer-solvent interactions, there is shear-thinning as η decreases with increasing shear velocity. The repulsive force (ΔF repulsive) due to interacting solvent and polymer between upper and lower walls increases with shear. Hence, the adhesion force decreases. When wall-solvent interaction is repulsive, the normal force between the walls is attractive (ΔF attractive) and decreases with shear, irrespective of the nature of wall-polymer and polymer-solvent interaction. Here also, the adhesion between the walls decreases with shear.

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Stochastic Relaxation Dynamics of a Feshbach coupled Atomic-Molecular Bose-Einstein-Condensates (BEC)

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Atomic and molecular bosons are weakly coupled to one another via Feshbach detuning in the usual Bosonic-Josephson-Junction (BJJ). Here, we study the imbalance between atomic and molecular bosons as a component of the Bloch vector. If coupling strength and detuning between the atomic and the molecular bosons are corrupted by Gaussian White Noise (GWN) then we obtain the relaxation dynamics of the Bloch vector to a stable equilibrium point. In this case, the relaxation rates in the Mean-Field (MF) method are lower or higher than Bogoliubov-Born-kirkwood-Yvon (BBGKY) hierarchy depending on the strength of the correlation between the Bloch vector components. Besides this, the particle localization shows a jump from a molecular heavy state to an atomic heavy state for critical detuning in the absence of noise. This sharp jumping point is spread out in the presence of noise.

Bond Percolation in Distorted Lattice

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Bond percolation is a probabilistic model used to study the formation of clusters in a network or lattice. This work exhibits a Monte-Carlo study on bond percolation using Newman-Ziff algorithm in distorted square and triangular lattices, where each site of the lattice is dislocated symmetrically and randomly from their regular position by a tunable parameter alpha. In this model, one bond is considered to be occupied only if the distance between two sites of the corresponding bond is less than the desired value and this desired value is known as connection threshold. It is observed that the percolation threshold always increases with distortion if the connection threshold is greater than or equal to lattice constant. On the other side, the percolation threshold always decreases with the connection threshold if the distortion parameter is greater than zero. Also we estimate the value of the critical connection threshold for different values of the distortion parameter.

Intermittent motion and strategies: collective order and transport optimization in active Brownian particles

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This project examines the collective and individual dynamics of particles alternating between "motile, aligning" (Active) and Brownian (Passive) states. This intermittent dynamics framework, relevant across various scales from bacteria to animals and artificial active systems, allows us to probe key transport properties and effective diffusivity. Our analysis reveals signatures of a phase transition in the system, where the global polarization—a measure of collective alignment—exhibits non-zero values below a critical active-to-passive switching rate. Additionally, we predict that with similar mean rate of energy expenditure, system with intermediate switching rates achieve almost equal efficiency compared to the incessantly active particles. These findings yield implications for both natural and engineered systems, especially concerned with target searching in a heterogenous environment.

An ab initio information-theoretic approach to proteins and protein-ligand interactions

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We propose an ab initio approach grounded in physical and information-theoretic principles for studying proteins associated with distinct signaling states. We introduce a de novo measure called protein residue information (PRI), which incorporates details of interactions between every pair of atoms both within and across all residues of any given protein. To determine PRI, we first formulate a method to calculate the intrastate and interstate entropy of every residue. Intrastate entropy can be determined for any given protein. Interstate entropy is calculated pairwise for proteins possessing more than one state. We analyse twenty-eight distinct pairs of proteins, from ten different classes. PRI successfully identifies important residues displaying both significant and subtle conformational changes bearing influence with respect to itself and all other residues. The identified residues exhibit influential roles in diverse performative features of proteins like stability, allostery, signaling, etc. PRI successfully recovers reported experimental results and predicts important roles for many hitherto unstudied residues. We further demonstrate that interstate entropy readily identifies residues that undergo higher conformational changes. The approach suffers neither from demanding computational expense nor from limitations of cutoff distance.

What is the Euclidean dimension of Ising Ferromagnetic Hollow Cube?

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The equilibrium and transient properties of magnetisation in the Ising ferromagnetic hollow cube (or cubic shell) have been extensively studied using Monte Carlo simulation. Although geometrically the Euclidean dimension of the hollow cube is three, interestingly, the Ising ferromagnetic cubic shell or hollow cube undergoes ferromagnetic phase transition at a temperature which is very close to that for two-dimensional Ising ferromagnet. Surprisingly, the Ising ferromagnetic hollow cube exhibits a anomalous (neither exponential nor stretched exponential) magnetic relaxation behaviour, instead of exponential relaxation as usually observed in the two and three dimensional Ising ferromagnetic systems. The external field dependence of meta-stable lifetime is thoroughly investigated and here also, the hollow cube behaves more likely a two-dimensional object as found from statistical analysis and comparison with Becker-Döring prediction of classical nucleation theory, showcasing three distinct regime, i.e. (i) strong field regime, (ii) coalescence regime and (iii) nucleation regime.

The effect of ZnO nanoparticle on the conformational changes of the α-synuclein molecule

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α-Synuclein (αS) is an intrinsically disorder protein involved in Parkinson's disease (PD) and is prone to form aggregates that are typically pathological [1]. The αS monomer loses its ordered or fixed 3D canonical structure during aggregation [2] and follows coil like structure. In a recent experimental study [3], the ZnO nanoparticle (ZnONP) interface has shown a direct effect on the conformation changes of αS and it may be used as a potential therapy for amyloidosis of αS. However, it has not been studied in detail how ZnONP affects on the conformational changes of the αS molecule. In this context, we use all-atom molecular dynamics (MD) simulation for 1μs to investigate microscopically the effect of the ZnONP on the conformational changes of the αS molecule. In MD, we take a 4 nm diameter ZnONP and an αS monomer (PDB id-1XQ8). Our result shows that the presence of ZnONP reduces the fluctuation of some residues of the αS molecule. Secondary structure analysis reveals that the percentage of coil conformation in the αS monomer decreases in presence of the ZnONP. The conformational thermodynamics calculation shows that the presence of the ZnONP stabilizes and orders the αS molecule.

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Interplay of particle and crystal symmetries in the discrete plastic crystal phase in entropic crystals

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Entropy-driven self-assembly facilitates the transition of disordered systems into or- dered structures, with entropy serving as the only driving force. As a robust model for such assembly, a system comprising rigid anisotropic convex polyhedra, governed solely by hard interactions, offers insight into particle orientational behavior, with the geometric centers of particles maintaining crystalline structures. Despite in- herent disorder within crystal unit cells, wherein translationally connected particles exhibit different orientations, a distance independent strong correlation emerges, re- sulting in a few conserved orientational quantities within the system. The discrete plastic crystal phase can be distinguished from the random orientationally disordered phase i.e., plastic crystal and orientatioally ordered phase. The particle point group symmetry possessing fewer rotational symmetry operations than the crystallographic point group symmetry yields a finite number of unique orientations, with almost equal population densities, maintaining specific orientational differences among them until the phase persists.

Revisiting the stability of the ordered flocking phase in the active Potts model

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Polar flocks are commonly observed in various active matter systems and have been considered robust to fluctuations. However, recent studies suggest that liquid polar flocks in active systems with discrete symmetry are metastable. In this work, we revisit the active Potts model (APM) to investigate the stability of the ordered flocking phase. Our findings indicate that the ordered phase in APM is metastable due to droplet excitation, and large spontaneous fluctuations can also destabilize the ordered flocks, akin to the active Ising model (AIM).

Phase transitions and Critical Behaviour in the classical XY ferromagnets with random anisotropy: A Monte Carlo study

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We investigate the three-dimensional anisotropic classical XY ferromagnet using extensive Monte Carlo simulations based on the Metropolis single spin-flip algorithm. We study the magnetization (M) and susceptibility (χ) as functions of temperature. For constant anisotropy, the ferro-para phase transition occurs at a higher temperature compared to the isotropic case, with increasing anisotropy strength leading to higher ordering temperatures. Conversely, in the presence of random anisotropy, the system orders at lower temperatures as the width of the anisotropy distribution increases, regardless of the distribution type (uniform, Gaussian, or bimodal). Phase boundaries for random anisotropy are presented, and critical exponents for the scaling laws $M \sim L^{-\beta/\nu}$ and $\chi \sim L^{\gamma/\nu}$ are estimated through finite-size analysis.

Directed Transport of Active Brownian Particles in a 3D Oscillatory Corrugated Channel

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This work explores the dynamics of active Brownian particles (ABPs) inside infinitely extended, three-dimensional, corrugated channels subjected to symmetric temporal oscillations. The stochastic Euler method is used to solve the overdamped Langevin equations that model particle movement. In order to study the impact of varying oscillation frequency, amplitude, translational diffusivity, and rotational diffusivity on particle mean velocity and effective diffusion, we utilize dynamic sliding reflection boundary conditions to confine the particles. The findings indicate that the resonance effect that increases directed motion is caused by particle transport, which is most effective at moderate oscillation frequencies. Particle activity and boundary oscillation motion interact to produce an effective diffusion peak at specific frequencies and amplitudes. Additionally, this work identifies the optimal range of translational diffusivity at which effective diffusion is at its smallest. These findings have significant implications for microfluidic device design, particularly in applications like targeted drug delivery and lab-on-chip systems. The study offers valuable insights into the entropic transport mechanisms of ABPs in oscillatory confined environments.

Spatially correlated motion across melting of two-dimensional Gaussian-core particles

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We study the dynamics of particles interacting via the Gaussian core model (GCM) across melting in pure and disordered two-dimensional (2D) systems. Intriguing signatures of cooperative motion of particles in string-like paths are found at low temperatures. Such a motion is common to glasses and supercooled liquids but we realize them in equilibrium phases, even in a pure system. We explore the interplay of such motion and impurities and report their repercussions on various spatiotemporal correlations. In particular, we find that such cooperative motion causes a departure from the diffusive dynamics, causing slow relaxation at low to intermediate temperatures.

Persistent Active Fluids

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Non-reciprocity and microscopic gyration

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Influence of Nanoparticle Shape on Polymer Flow and Wetting Dynamics: A Molecular Dynamics Approach

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Anomalous collective diffusion of interacting run-and-tumble particles

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We characterize the collective motion of interacting run-and-tumble particles (RTPs) by calculating the bulk-diffusion coefficient in two minimal model systems, for arbitrary density ρ and tumbling rate γ, and offer a generic mechanism to account for the early-time anomalous relaxations. In the strong persistence limit of γ <<1, the fascinating interplay between persistence and interaction is quantified in terms of two length scales - “mean free path” and persistence length l_p = v/γ, with v being the self-propulsion speed. Indeed, we show that the bulk-diffusion coefficient has a scaling form D(ρ; γ) = D(0)F (ρv/γ), where D(0) is proportional to the diffusivity of noninteracting particles; the scaling function F (ρv/γ) is calculated analytically for one model and numerically for the other. In this limit, we find that the bulk-diffusion coefficient varies as a power law in a wide range of density : D ~ ρ^{−α}, with exponent α gradually crossing over from α = 2 at high densities to α = 0 at low densities. As a result, the density relaxation is governed by a nonlinear diffusion equation with anomalous spatiotemporal scaling that can be ballistic in certain regimes. Our arguments, as demonstrated in simulations, are rather generic, being independent of dimensions and microscopic details.

Einstein - Smoluchowski theory of Brownian motion

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The Brownian motion of a particle will be discussed in the light of Einstein-Smoluchowski theory to find the time dependent probability of finding the particle at any position. The time dependence of root mean squared displacement will be calculated.

Existence of Limit Cycles and Fixed Points in Bacterial Respiration: A Stochastic and Experimental View

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In modern microbiology, understanding the intricate dynamics of bacterial respiration is crucial for unraveling the complexities of bacterial behavior and lifestyle. This study explores bacterial respiration by analyzing the Fairen-Velarde coupled nonlinear differential equations, introducing stochasticity through random noise to capture the inherent variability in the system. We also experimentally validate the deterministic predictions of the Fairen-Velarde model using E. coli bacteria, demonstrating the existence of limit cycles and fixed points in bacterial respiration. Our findings provide a unique stochastic and experimental perspective on the complex regulatory mechanisms driving bacterial metabolic processes.

Negative Temperature and it's experimental realisation

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Negative Temperature, a counterintuitive concept in classical thermodynamics, describes systems where higher energy states are more populated than lower ones. It is a non equilibrium phenomena that arises when magnetic dipoles are in opposite to the direction of magnetic field. Experimental evidence of negative temperature has been observed in many systems like nuclear spin systems, atoms in a magnetic trap etc.