125th STATISTICAL MECHANICS CONFERENCE

SHORT TALK SCHEDULE

SESSION A

A1: Daniel Swartz, MIT
Title: Morphological Outcomes of Spatial Expansion in Microbial Colonies
Coauthors: Hyunseok Lee, Kirill Korolev, Mehran Kardar
Abstract: Spatial expansion has played a role in the evolution of nearly all species. Microbial colonies in a Petri dish provide a controllable way to assess the consequences of range expansion on the fates of the constituent strains. We use a combination of analytic theory and computational modelling to describe the different outcomes of this spatial competition, and quantify how the morphology of the resulting colony is shaped by dispersal and competition. We find that the morphology of microbial colonies is not only indicative of competitive viability but is also influenced by the symmetry of their habitat. This morphology can be leveraged to promote coexistence among strains.

A2: Debbie Zhuang, MIT
Title: Stability Theory of Phase Separating Many Particle Populations
Coauthors: Martin Z. Bazant
Abstract: Only macroscopic level bath control can be exerted on a system that contains many reactive particles, which is complicated by the large number of degrees of freedom in the system. When introducing phase separating thermodynamics to such a system, the individual particle thermodynamics introduces more convolution into the problem. Bath potential control over such a system is found to decouple all particles to single particle stability. However, the system exhibits different behavior when under net reaction control. We attempt to extract the stability of this system using degenerate matrix perturbation methods. Net reaction control returns modified eigenvalues, with eigenvectors indicating coupling between the particles induced by reaction control through the bath. Such analyses can provide insight into engineering control of reactive systems such as lithium ion batteries.

A3: Michael Li, MIT
Title: Domain Switching Instabilities in Heterogeneous Ferroelectric Microstructures
Coauthors: Martin Z. Bazant
Abstract: In ferroelectric thin film devices, complex electrostatic, chemical, and mechanical coupling of various domains leads to non-linear switching dynamics. These materials undergo phase transformations induced by applied electrostatic potentials, which can propagate to nearby domains. To analyze this problem, we simplify the system to a two-phase structure with heterogeneity in the free energy functional to determine the competition between bulk and

interface. We find that surface tension at grain boundaries greatly influences the phase stability. Through this approach, regions of the microstructure that trigger device switching are identified, which is critical in predicting thin-film device performance.

A4: Guilherme de Sousa, University of Maryland, College Park
Title: Using filters to study stochastic continuous quantum measurements
Abstract : My work is focused on quantum continuous feedback. The outcome of a quantum measurement is stochastic by nature, and we model a continuous measurement using white Gaussian noise to describe the measurement outcome. Recently, I've been focusing on studying how we can apply linear filtering to decrease the noise of the measurement outcome and have a more tractable signal. Using a low-pass filter, we can map the problem to the evolution of an Ornstein–Uhlenbeck process. More general filters can sometimes be modeled using coupled Ornstein-Uhlenbeck processes or more complex stochastic equations.

A5: Niranjan Sarpangala, University of Pennsylvania
Title: Designing truss network based mechanical metamaterials using a spectral method
Coauthors: Sean Fancher, Prashant K. Purohit and Eleni Katifori
Abstract : Mechanical truss structures are widely used in civil engineering, primarily for their remarkable stability at low material cost. Synthesis of materials with such structures on the sub-millimeter scale is now possible because of recent breakthroughs in additive manufacturing technology. Such efforts have indicated that the structure of the materials can impact their function. However, a proper fundamental understanding of this structure-function relation is necessary to fully exploit the advancements in manufacturing technology. Here we explore the dynamics of elastic networks of truss structures and aim to design networks with distinctive mechanical properties. We use a spectral method, previously developed within our group and analyze the dynamics of truss networks in the Fourier domain. Our goal is to design networks with specialized features, such as those that can serve as acoustic filters or protect designated areas within the material from mechanical shocks. This research has implications for the synthesis of mechanical metamaterials, particularly in areas like packaging and acoustic.

A6: Joshua Chiel, University of Maryland
Title: Fast Thouless Pumps
Coauthors: Christopher Jarzynski, Jay Sau
Abstract : Thouless pumps produce topologically robust charge transport at the price of adiabaticity. Shortcuts to adiabaticity methods circumvent this slowness requirement by adding energy to the system in a structured way to achieve a speed up.

A7: Moallison Ferreira Cavalcante, University of Maryland Baltimore County
Title: Nano-welding at minimal dissipation
Abstract: Recent developments in nanotechnology and nano-electronics necessitate the design of

optimal design strategies. For instance, the "welding" of nano-wires needs to be facilitated at minimal material strain, or more thermodynamically speaking, at the least amount of dissipation. As a simple, pedagogical, and mathematically tractable example of such nano-welding, we consider two XX spin chains with open boundary conditions, that are to be joined at one end. We model the "welding" as the turning-on of a coupling term between the end-points of the spin chains. To analyze the energetics of the process, we express the excess or dissipated work by means of perturbation theory. As a main result, we derive the optimal control protocol for turning on the interaction that minimizes the excess work.

A8: Amer Al-Hiyasat, MIT
Title: Thermalization in overdamped linear systems
Coauthors: Amer Al-Hiyasat*, Julien Tailleur
Abstract: We consider the dynamics of a zero-temperature tracer particle coupled to a bath of overdamped particles at temperature T. We study the conditions under which the tracer particle thermalizes and approaches an equilibrium dynamics at the same temperature as the bath. Our findings show that several well-known models of thermalization in linearly coupled Hamiltonian systems fail to describe thermalization in overdamped systems. This work has implications for the simulation of tracer dynamics in colloidal baths.

A9: Jaeuk Kim, Princeton University
Title: Extraordinary Electromagnetic Properties of Disordered Stealthy Hyperuniform Layered Media
Coauthors: Salvatore Torquato
Abstract: Disordered stealthy hyperuniform (SHU) dielectric composites exhibit novel electromagnetic wave transport properties in two and three dimensions, but much less is known about such one-dimensional (1D) or layered media. From exact nonlocal strong-contrast expansions of the effective dynamic dielectric constant tensor that treat general three-dimensional two-phase composites with arbitrary structural symmetries, we extract an approximation formula suited for general layered media. This formula depends on the microstructure via the spectral density, and we apply it to estimate the effective dielectric constant for SHU variants. In particular, we predict that 1D SHU media are perfectly transparent (trivially implying no Anderson localization, in principle) within finite wavenumber intervals. We validate that the resulting predictions are very accurate well beyond the long-wavelength regime by showing good agreement with the finite-difference time-domain (FDTD) simulations. The high predictive power of our formula implies that higher-order contributions are negligibly small. Indeed, we prove that such media are exactly transparent for such intervals at the second- and third-order terms in the expansion. Thus, there can be no Anderson localization within the predicted perfect transparency interval in 1D SHU media in practice because the localization length (associated with only possibly negligibly small higher-order contributions) should be very large compared to any practically large sample size. [1] J. Kim and S. Torquato, Optica, 10 965–

972 (2023) [2] J. Kim and S. Torquato, Opt. Mater. Express, under review, (2023)

A10: Peter Morse, Princeton University
Title: The densest sphere packing in Fourier space is always a Bravais lattice
Coauthors: Paul Steinhardt, Sal Torquato
Abstract: Stealthy hyperuniform systems are characterized by a structure factor S(k) which is precisely zero within a finite "exclusion region" 0sely zero for distances less than the particle diameter. In light of this, stealthy hyperuniform systems can be exactly characterized as hard spheres in Fourier space. In the study of real space hard spheres, it has been fruitful to interrogate how the maximum density and the onset of order through freezing proceed with increasing spatial dimension. Because stealthy hyperuniform systems have a fundamental constraint on their freezing transition which limits the density of disordered structures, these questions can be answered more precisely in Fourier space. Due to the lower bounds on crystal density, we prove that the densest Fourier space hard sphere system is that of a Bravais lattice in all dimensions. The same cannot be said of real space hard sphere systems, wherein it has not yet been thoroughly proven whenter Bravais lattices, non-Bravais lattices, or disordered systems are the densest sphere packings as spatial dimension tends towards infinity.

A11: Sangyun Lee, University of Maryland
Title: QNEE, a quantum entropy estimator based on an entropy inequality
Coauthors: Hyukjoon Kwon, Jae Sung Lee
Abstract: Estimating entropy production without detailed information about the system is difficult because it is under the curse of dimensionality. Over the past decade, various stochastic entropy inequalities have been employed to estimate stochastic entropy production. These methodologies have shown great accuracy while mitigating the curse of dimensionality. One of the methods is unsupervised learning with the cost function based on an entropy inequality. Similar inequality can be found for quantum entropy. In this research, we present how to estimate quantum entropy using a neural network and a quantum circuit. We verify Quantum Neural Entropy Estimator (QNEE) on the estimation of the XXZ model's entanglement entropy. We found that QNEE can efficiently classify the phase of the quantum system.

A12: Todd Gingrich, Northwestern University
Title: Quantifying Rare Events in Stochastic Reaction-Diffusion Dynamics Using Tensor Networks
Coauthors: Schuyler Nicholson
Abstract: The interplay between stochastic chemical reactions and diffusion can generate rich spatiotemporal patterns. While the timescale for individual reaction or diffusion events may be very fast, the timescales for organization can be much longer. That separation of timescales makes it particularly challenging to anticipate how the rapid microscopic dynamics gives rise to macroscopic rates in the nonequilibrium dynamics of many reacting and diffusing chemical

species. Within the regime of stochastic fluctuations, the standard approach is to employ Monte Carlo sampling to simulate realizations of random trajectories. I will present an alternative numerically tractable approach to extract macroscopic rates from the full ensemble evolution of many-body reaction-diffusion problems. The approach leverages the Doi-Peliti second-quantized representation of reaction-diffusion master equations along with compression and evolution algorithms from tensor networks. Because we directly work with ensemble evolutions, we crucially bypass many of the difficulties encountered by rare event sampling techniques—detailed balance and reaction coordinates are not needed.

A13: Tim Halpin-Healy, Barnard / Columbia Univerity
Title: KPZ Exponents
Abstract: I report on recent work dovetailing Real-Space Renormalization Group (RSRG) & field-theoretic Dynamic RG approaches w/ the goal of pinning down the key scaling index of the many-dimensional KPZ universality class.

SESSION B

B1: Pradeep Natarajan, MIT
Title: A mechanism for arrest in coarsening by active reactions
Coauthors: Andriy Goychuk, Mehran Kardar, Arup Chakraborty
Abstract: Cells are a bag of biomolecules that are spatially organized to carry out function. Recent literature suggests that interactions between biomolecules such as proteins and RNAs can make them form like droplets called biomolecular condensates. This happens through a phase separation mechanism just like oil and water. If these condensates are close to equilibrium, we would eventually expect them to coarsen into one large droplet. However, imaging studies in cells reveal that there are persistently many droplets of a typical size. Why does this happen and what sets the droplet size? We suggest that non-equilibrium mechanisms are at play. We construct a simple phase-field model of biomolecular condensates containing two species: proteins and RNAs. This model incorporates the physics of protein phase separation, RNA-protein interactions, and RNA production catalyzed by the proteins. By linearizing this model in Fourier space we derive an expression for the growth rate of the Fourier modes of the protein concentration field. We show that the growth rate has an additional term that arises due to the coupling of the protein dynamics to the RNA dynamics involving diffusion-production-degradation by the RNA-protein interactions. This term leads to an effective long-range interaction kernel between the protein that arrests coarsening and leads to a typical droplet size. We also predict that this droplet size should increase upon decreasing RNA production rate, which is also confirmed by biological experiments.

B2: Jiming Zheng, UNC Chapel Hill
Title: Calibrate Time with Arbitrary Markov Process
Coauthors: Zhiyue Lu
Abstract: Brownian clocks with oscillating probability distributions can be used to calibrate time. Examples include chemical oscillations and biological circadian clocks. Here, we argue that any Markov process, even equilibrium ones and ones without cyclic states, can calibrate time. In contrast to previous approaches that focus on the probability distributions of states, we focus on the ensemble of stochastic trajectories from a Markov system, which includes more information than the state distributions. We derive a universal quantity that characterizes a Markov process's ability for time calibration and show that it is entirely captured by the dynamical activity of the Markov process, regardless of the detailed balance condition or the complexity of the Markov process.

B3: Zhongmin Zhang, UNC Chapel Hill
Title: On the non-equilibrium design of single-molecule computation
Coauthors: Zhiyue Lu

Abstract: Living matter, such as cells or biomolecules, can respond to time-varying complex environments and perform functions. We design a molecule that can recognize, memorize, and respond specifically to temporal patterns of a changing environment. Moreover, it can be steered arbitrarily far away from equilibrium by temporal protocols. The smart molecule is demonstrated by an Ising-model-like linear polymer chain consisting of N foldable units with 2^N possible configurations, with its end-to-end distance under external temporal control. We propose a kinetic frustration design principle of energy landscapes, which allows the evolution of the molecule's most probable configuration (i.e., the dominant configuration) to be simplified into three simple logical rules. This allows us to obtain nonequilibrium protocols to steer the molecule into nonequilibrium distributions with any desired dominant configuration out of the 2^N configurations. Lastly, the molecule's response to the external control mimics a computing device, specifically, a deterministic finite automaton.

B4: Matthew Marko, Marko Motors LLC

Title: Utilizing the Van der Waals forces of a non-ideal working fluid to boost the thermodynamic efficiency of a practical Stirling cycle heat engine

Abstract: A novel variation of the Stirling thermodynamic heat engine cycle was designed and patented. This variation is unique in that instead of an ideal gas working fluid, it utilizes a real fluid, subjected to the Van der Waals intermolecular attractive force. When there is a heat engine cycle with constant-temperature (isothermal) compression and expansion (such as in a Carnot or Stirling cycle heat engine) utilizing a non-ideal working fluid, the Van der Waals intermolecular attractive force will both beneficially reduce the mechanical work input at the cold isothermal compression stage, as well as detrimentally reduce the mechanical work output at the hot isothermal expansion stage. It is observed from the empirical equations of state for real fluids that the Van der Waals intermolecular attractive forces of a real fluid, in addition to being stronger with density, are also stronger with colder temperatures. As a result, the beneficial reduction in mechanical work input will exceed the detrimental reduction in mechanical work output, yielding a net increase in the work output, and theoretically boosting the thermodynamic efficiency of this macroscopic heat engine to exceed that of the Carnot efficiency limit of an ideal gas! Utilizing direct measurements of the temperature drop due to the Joule-Thomson effect of a real fluid (carbon dioxide), an accurate empirical equation for the true internal energy of a real fluid was obtained and utilized in the practical design of such a novel Stirling cycle heat engine, which could have many valuable applications in the generation of carbon-neutral solar energy generation! https://www.nature.com/articles/s41598-022-11093-z US-11,078,869 "Condensing Stirling cycle heat engine", 2021-08-03

B5: Emery Doucet, University of Maryland Baltimore County

Title: Quantum Darwinism meets Quantum Demons – Emergence of Classical Reality in a Complex Universe

Coauthors: Sebastian Deffner

Abstract: Quantum Darwinism provides a framework to understand the emergence of an objective and classical reality in a fundamentally quantum world. However, it is not currently known what properties a general Hamiltonian must have to support classicality. A recent work by Duruisseau, Touil, and Deffner [1] has made an important step in this direction by classifying generic qubit Hamiltonians. In this talk, I will discuss the progress we have made in generalizing this result to a wider range of system Hamiltonians and environment interactions. We find that the zoo of Hamiltonians which can support the emergence of objectivity is larger and more diverse for more complex systems. A taxonomy of Hamiltonians classified according to their ability to support quantum Darwinism will be a useful tool to guide analyses of quantum-to-classical transitions in many contexts, as for instance in minimal models of Maxwell's demon. [1] arXiv:2309.03299

B6: Debankur Bhattacharyya, University of Maryland, College Park
Title: Continuous measurement and feedback-control for deterministic and diffusive flows: A master equation formalism
Coauthors: Long Him Cheung, Guilhereme De Sousa, Christopher Jarzynski
Abstract: I will present a stochastic description of classical feedback-controlled systems modeled using a Fokker Planck master equation similar to one derived recently for quantum feedback-controlled systems [Phys. Rev. Lett., 129, 050401 (2022)]. The control parameter is a classical variable that evolves based on measurements performed on the system of interest. The master equation describes the evolution of the joint probability distribution of the state of the system and the control parameter. This formalism accounts for measurement errors, time delay and nonlinear feedback protocols. I will also present possible applications of this equation relating to feedback controlled dynamics of overdamped Brownian particles.

B7: Charles Maher, Princeton University
Title: Hyperuniformity of maximally random jammed packings of hyperspheres across spatial dimensions
Coauthors: Yang Jiao, Salvatore Torquato
Abstract: The maximally random jammed (MRJ) state is the most random (i.e., disordered) configuration of strictly jammed (mechanically rigid) nonoverlapping objects. MRJ packings are hyperuniform, meaning their long-wavelength density fluctuations are anomalously suppressed compared to typical disordered systems, i.e., their structure factors S(k) tend to zero as the wave number |k| tends to zero. Here we show that generating high-quality strictly jammed states for Euclidean space dimensions d = 3, 4, and 5 is of paramount importance in ensuring hyperuniformity and extracting precise values of the hyperuniformity exponent $\alpha > 0$ for MRJ states, defined by the power-law behavior of $S(k) \sim |k|^{\alpha}$ in the limit $|k| \to 0$. Moreover, we show that for fixed d it is more difficult to ensure jamming as the particle number N increases, which results in packings that are nonhyperuniform. Free-volume theory arguments suggest that the ideal MRJ state does not contain rattlers, which act as defects in numerically generated packings. As d increases, we find that the fraction of rattlers decreases substantially. Our analysis of the

largest truly jammed packings suggests that the ideal MRJ packings for all dimensions d = 3 and greater are hyperuniform with $\alpha = d - 2$, implying the packings become more hyperuniform as d increases. The differences in α between MRJ packings and the recently proposed Manna-class random close packed (RCP) states, which were reported to have $\alpha = 0.25$ in d = 3 and be nonhyperuniform ($\alpha = 0$) for d = 4 and d = 5, demonstrate the vivid distinctions between the large-scale structure of RCP and MRJ states in these dimensions. Our paper clarifies the importance of the link between true jamming and hyperuniformity and motivates the development of an algorithm to produce rattler-free three-dimensional MRJ packings.

B8: Murray Skolnick, Princeton University
Title: Quantifying phase mixing and separation behaviors across length and time scales
Coauthors: Salvatore Torquato
Abstract: Phase mixing and separation phenomena abound in a multiplicity of diverse material systems including composites, alloys, granular media, complex fluids, and biological tissues. While characterizing phase mixing is critical to understanding material microstructure formation, manufacturing methods, and physical properties, previous mixing metrics are only valid for special systems and fail to detect changes in mixing with respect to length scale, not to mention time scales. To improve upon the current state-of-the-art, we introduce and study a broadly applicable mixing metric that leverages the hyperuniformity concept, demonstrating that it provides the first unifying framework for systematically ranking and classifying mixing in materials across length and time scales. This task is accomplished by applying our metric to a diverse set of real and simulated material microstructures with varying degrees of order/disorder as well as distinct phase geometries and topologies. Our metric provides physically intuitive rankings of mixing in these example systems and is highly-sensitive to their salient dynamical features, including phase coarsening, separation, and transitions. We expect that our mixing metric can also be used to inform the design and discovery of materials with prescribed length- and time-dependent phase mixing or separation behaviors.

B9: Sunghan Ro, MIT
Title: Diffusion with center of mass conservation
Coauthors: Jung Hoon Han, Ethan Lake
Abstract: Diffusion in systems of classical particles with dynamics that conserve the total center of mass will be presented. Interestingly, in d dimensions, the dynamic exponent shifts to z = d+4, and the equilibrium distribution exhibits exponential localization in the presence of a hard wall. We will also demonstrate that similar phenomena arise in dynamics conserving higher moments of the density.

B10: Haina Wang, Princeton University
Title: Hyperuniformity in Free and Interacting Ground-State Fermi Gases

Coauthors: Rhine Samajdar, Salvatore Torquato

Abstract: The Fermi gas model is the most fundamental quantum-mechanical model for fermions and provides excellent theoretical framework for electrons in metals and semiconductors. Despite numerous theories describing the pair correlation function $g_2(r)$ and structure factor $S(k)$ for Fermi gases, there has been limited analytical study on the small-wavevector behaviors of the pair statistics. Using the random phase approximation and the Hubbard approximation, we derive analytical asymptotic expressions for the small-k behaviors of total and spin-resolved structure factors for quasi-1D, 2D and 3D fermi gases, as a function of the interaction parameter r_S and the polarization factor ζ. We find that free fermions, partially polarized interacting fermions and fully polarized fermions form three distinct ``phases'' characterized by different hyperuniform properties of the structure factors. Remarkably, the partially polarized interacting fermions are highly unusual multihyperuniform states, in which the total configuration is of a higher hyperuniformity class than the individual spin components. Our asymptotic expressions via the Hubbard model agree well with numerical results obtained from the Singwi-Tosi-Lobo-Land formalism. To study the limitation of the pair correlations to capture Fermi-gas structures, we determine classical many-body systems that correspond to 2D and 3D free-fermion pair statistics, and find that significant differences emerge in the three-body statistics between the equivalent quantum and classical states. Our work enables one to develop more accurate density functional theories for fermionic systems and reveal novel pathways to create exotic hyperuniform and hyperuniform materials via quantum states.

B11: Andriy Goychuk, MIT

Title: Sharp interface theory of active condensate dynamics

Coauthors: Leonardo Demarchi, Ivan Maryshev, Erwin Frey

Abstract: Active biomolecular condensates, in which enzymes catalyze chemical reactions among their substrates, can show non-equilibrium behavior such as self-propulsion. To quantitatively explain these dynamics, we have developed a two-step model reduction scheme. First, assuming the droplet shape and velocity as known, we infer the enzyme currents and chemical potential profile in a model-independent way. Then, by keeping track of the flux of energy, we draw a phase portrait which selects a thermodynamically consistent value for the droplet speed. Interestingly, our theory predicts that liquid-like droplets have much higher effective mobility than solid-like condensates.

B12: Federica Ferretti, MIT

Title: Universal characterization of epitope immunodominance from a multi-scale model of clonal competition in germinal centers

Coauthors: Mehran Kardar

Abstract: We introduce a simple disordered population dynamics model for affinity maturation

-- the evolutionary process through which B cells acquire specificity upon encounter of a novel foreign pathogen -- which aims to capture the multi-scale organization of the B cell population in a germinal center. Within this mathematical framework, we study the competition among subpopulations of B cell clones targeting different antigen epitopes, and construct an effective 'immunogenic' space where epitope immunodominance relations can be universally characterized. We study how combinations of antigens with variable and conserved domains results in a parametric exploration of this space, and identify general principles for the rational design of two-antigen cocktails.

B13: Gerald Goldin, Rutgers University
Title: Group theoretical predictions of anyonic quantum kinematics
Coauthors: Hongyi Shen
Abstract: One of us (GG) has proposed (with David H. Sharp, Los Alamos Nat'l. Lab.) that the unitary representations of a single infinite-dimensional group describe all possible quantum kinematics of matter in physical space M. When M in two-dimensional, this framework yielded (with Ralph Menikoff, LANL) an early prediction of anyon (braid) statistics, and the first prediction of nonabelian anyons. We have found that in two-space, additional "internal" quantum phases are predicted by representations describing particles or excitations having internal structure -- dipole, quadrupole, and higher multipole configurations. One may think of such systems as tightly bound composite particles.