119^{th} STATISTICAL MECHANICS CONFERENCE

SHORT TALK SCHEDULE

SESSION A

A1: Maxim Zyskin, **Rutgers & Nottingham**
Elasticity of defective crystals

Abstract: In continuum theory of perfect crystals, SL(3,Z) lattice symmetry implies under quite general assumptions that stress tensor is pressure. This need not be the case for recently investigated by us types of defective crystals, which have different symmetries.

A2: Ralph Chamberlin, **Arizona State University**
Characterizing the correlations that cause equilibrium fluctuations to deviate from behavior predicted by Boltzmann's factor

Abstract: We use experiments, theory, and computer simulations to investigate discrepancies between microscopic dynamics and standard statistical mechanics. Theoretically, Boltzmann's factor is based on weak thermal contact to an effectively infinite heat reservoir, unlike fluctuations of individual particles that are governed by direct interactions with neighboring particles. I will focus on MD simulations showing that small "blocks" of particles inside much larger volumes may exhibit energy fluctuations that exceed the standard fluctuation-dissipation relation by an order of magnitude or more. Such anomalous energy fluctuations are found to coincide with enhanced correlations in the energies of neighboring blocks. We characterize these correlations as a function of time and distance, and argue that they are inconsistent with many measurements showing that the primary response of most substances involves nanometer-sized regions that are effectively uncorrelated. If time permits, I will discuss how a nonlinear correction to Boltzmann's factor can decorrelate neighboring regions, restore statistical mechanics as a description of local fluctuations, and provide a common explanation for several empirical formulas, including stretched-exponential relaxation, non-classical critical scaling, and 1/f noise.

A3: Duyu Chen, Princeton University
Coauthors: Enrique Lomba, Salvatore Torquato
Binary Mixture of Charged Colloids: A Potential Route to Synthesize Disordered Hyperuniform Materials

Abstract: Disordered hyperuniform materials are new, exotic class of amorphous matter that exhibit crystal-like behavior, in the sense that volume-fraction fluctuations are suppressed at large length scales, and yet they are isotropic and do not display diffraction Bragg peaks. These materials are endowed with novel photonic, phononic, transport and mechanical properties, which are useful for a wide range of applications. Motivated by the need to fabricate large samples of disordered hyperuniform systems at the nanoscale, we study the small-wavenumber behavior of the spectral density of binary mixtures of charged colloids in suspension. The interaction between the colloids is approximated by a repulsive hard-core Yukawa potential. We find that at dimensionless temperatures below 0.05 and dimensionless inverse screening lengths below 1.0, which are experimentally accessible, the disordered systems become effectively hyperuniform. Moreover, as temperature and inverse screening length decrease, the level of hyperuniformity increases, as quantified by the ``hyperuniformity index''. Our results suggest an alternative approach to synthesize large samples of effectively disordered hyperuniform materials at the nano scale under standard laboratory conditions. In contrast with the usual route to synthesize disordered hyperuniform materials by jamming particles, this approach is free from the burden of applying high pressure to compress the systems.

A4: Michael Kiessling, Rutgers University
Coauthors : Michael Kiessling and A. Shadi Tahvildar-Zadeh

On the Quantum Mechanics of a Single Photon

Abstract: We propose a relativistic quantum-mechanical wave equation for a single photon which is a direct analog of Dirac's relativistic wave equation for the electron. The equation is covariant under the full Lorentz group. It's solutions are bi-spinors of rank 2 with vanishing trace, elements of a complex Hilbert space. Most importantly: the photon wave equation gives rise to a conserved probability current which transforms properly under the Lorentz group, obeying Born's rule for finding a photon at a particular point in space. Einstein's relations between Energy and frequency, respectively momentum and wavelength, are obtained, and so is the usual dispersion relation for massless particles.

A5: Ronald Fisch

Scaling Behavior in the 3D Random Field XY Model

Abstract: We have performed Monte Carlo studies of the 3D random field XY model on $L \times L \times L$ simple cubic lattices with periodic boundary conditions, using a random field strength of h_r = 1.875, for $L = 64$ and $L = 96$. Results for the angle-averaged magnetic structure factor, $S (k)$ at $T = 1.00$ will be presented. At this temperature, the results indicate the existence of a logarithmic divergence of $S (k)$ as $k \to 0$, both for samples which are slowly cooled and also for samples which are slowly heated. This suggests that the lower critical dimension for long range order in this model is 3. It is expected that the methods used will be able to produce similar results for $L = 128$.

A6: Eugene Kolomeisky, University of Virginia

Nonlinear plasma waves in an electron gas

Abstract: The nature of traveling wave solutions to equations of hydrodynamics of a generic three-dimensional electron gas with parabolic dispersion law depends on whether the motion is subsonic or supersonic. Solitons representing localized depressions of the electrostatic potential and electron density are predicted to exist in the subsonic regime: at rest the solitons are dark while in motion they are grey. Two types of periodic waves are found in the supersonic regime: (i) smooth waves whose small amplitude limit is described by harmonic theory, and (ii) waves with sharp troughs and smooth crests of the potential with the electrons accumulating in the troughs.

A7: Douglas Abraham, University of Oxford

Coauthors : Anna Maciolek, Alessio Squarcini, Oleg Vasyliev

Recent exact results for fluctuation induced interactions

Abstract: We show how boundary fields can be used to control the sign of thermal Casimir forces and we also explain the strong asymmetry first noted by Evans and Stecki. Results on emergent long range forces will also be discussed. Refs: PRL 105, 055701; EPL 101(2):20006 (2013); PRL 113, 077204 (2014); Phys Rev E96, 042154 (2017).

SESSION B

B1: Sungchul Ji – Rutgers University
Planckian information is to Info-Statistical Mechanics what Boltzmann entropy is to Statistical Mechanics

Abstract: Traditionally, the dynamics of any N-particle systems in statistical mechanics is completely described in terms of the 6-dimensional phase space consisting of the 3N positional coordinates and 3N momenta, where N is the number of particles in the system [1]. Unlike the particles dealt with in statistical mechanics which are featureless and shapeless, the particles of importance in biology have characteristic shapes and internal structures that determine their biological properties. Particles in physics are completely described in terms of energy and matter (in the phase space) but the description of the particles in living systems require not only the energy and matter of the particle but also the genetic information carried by the particle, consistent with the information-energy complementarity (or gnergy) postulate discussed in [2, Section 2.3.2]. Thus, it seems necessary to expand the dimensionality of the traditional phase space to accommodate the information dimension, which includes the three coordinates encoding the amount (in bits), meaning (e.g., recognizability), and value (e.g., practical effects) of information [2, Section 4.3]. Similar views have been expressed by Bellomo et al. [3] and Mamontov et al. [4]. The expanded "phase space" would comprise the 6N phase space of traditional statistical mechanics plus the 3N information space entailed by molecular biology. Therefore, the new space (to be called the "gnergy space") composed of these two subspaces would have 9N-dimension as indicated in Eq. (1): Gnergy Space = 6N-D Phase Space + 3N-D Information Space (1) (Synchronic Space) (Diachronic Space) The study of information and energy is defined as info-statistical mechanics in 2012 [2]. In 2008, at the 100th meeting of this Conference [5], I reported the derivation of Equation (2) referred to as the Planckian Distribution Equation (PDE) from the blackbody radiation equation discovered by M. Plank in 1900 by replacing its universal constants and temperature with free parameters, A, B and C: y = A/(x+B)5/(eC/(x + B) – 1) (2) PDE has been found to fit almost all the long-tailed histograms we have analyzed so far in the fields of atomic physics, molecular biology, cell biology, neurophysiology, psychology, glottometrics (or quantitative linguistics), econometrics, cosmology [2, 6], and most recently social network science [7]. The deviation of PDE from a symmetric curve such as the Gaussian distribution function can be used as a measure of non-randomness and hence of order and information [4, 5]. There are two ways of quantifying the information content of PDE [6, 8]: Plankian information of the first kind: IPF = log2 [AUC (PDE)/AUC (GLE)] (3) Plankian information of the second kind: IPS = - log2 [(μ – mode)/σ] (4) where AUC = Area Under the Curve; GLE = Gaussian-like Equation whose rising portion approximates closely the rising portion of PDE, and μ and σ are, respectively, the mean and the standard deviation of the data set representable as a long tailed histogram that fits PDE. In contrast to the Boltzmann entropy which measures disorder (or disorganized complexity of Weaver [10]), the Planckian information defined by Equations (3) or (4) is thought to measure order (or the organized complexity [10]). The inseparable relation between energy and information that underlies "info-statistical mechanics" may be expressed by the following aphorism: "Information without energy is useless; Energy without information is valueless." References: [1] Tolman, R. C. (1979). The Principles of Statistical Mechanics, Dover Publications, Inc., New York, pp. 42-46. [2] Ji, S. (2012) Molecular Theory of the Living Cell: Concepts, Molecular Mechanisms, and Biomedical Applications. Springer, New York. [3] Bellomo, N., Bellouquid, A. and Harrero, M. A. (2007). From microscopic to macroscopic descriptions of multicellular systems and biological growing tissues. Comp. Math. Applications 53: 647-663. [4] Mamontov, E., Psiuk-Maksymowitcz, K. and Koptioug, A. (2006). Stochastic mechanics in the context of the properties of living systems. Math. Comp. Modeling 44(7-8): 595-607. [5] Ji, S. (2008). Modeling the single-molecule enzyme kinetics of cholesterol oxidase based on Planck's radiation formula and the principle of enthalpy-entropy compensation, in Short Talk Abstracts, The 100th Statistical Mechanic Conference, December 13-16, Rutgers University, Piscataway, N.J. [6] Ji, S. (2018). The Cell Language Theory: Connecting Mind and Matter. World Scientific Publishing, New Jersey. Chapter 8. [7] Navarro, J., del Moral, R., Gomez-Quintero, J. D., Bordonaba, D., Montero-Marin, J., Ji, S., and Marijuan, P. C. (2018). QUANTITATIVE SOCIOTYPE: Exploring the Social Structures and Communication Relationships around the Individual. Human Nature (in press). [8] Ji, S. (2018). RASER Model of Single-Molecule Enzyme Catalysis and Its Application to the Ribosome Structure and Function. Arch. Mol. Med. & Genetics. 1: 31-39. [9] Boltzmann distribution law. https://en.wikipedia.org/wiki/Boltzmann_distribution. [10] Weaver, W. (1948) Science and Complexity. American Scientist 36:536-544.

B2: Jaeuk Kim, Princeton University
Coauthor: Salvatore Torquato
A tiling method to construct disordered hyperuniform two-phase media

Abstract: Heterogeneous media are systems, comprised of different materials (or phases), and can have a wide range of effective physical properties by engineering spatial arrangement of phases. One special type of such systems is disordered hyperuniform (two-phase) heterogeneous media; they behave like liquids in that they are statistically isotropic without Bragg peaks, and yet, like crystals, suppress density fluctuations at large length scales. There has been a surge of interest in those systems because of their exotic physical properties, such as sizable complete photonic band gaps and nearly optimal transport properties. While many experimental and computational methods have been developed to generate disordered hyperuniform two-phase media, there has been no method based on the constraints in local structures. Here, we propose a new construction method via local geometric constraints in d-dimensional Euclidean space. This scheme is a generalization of a work of Gabrielli and his colleague [Gabrielli, et al., Phys. Rev. E 77, 031125 (2008)]. Starting from a Voronoi tessellation of a given nonhyperuniform particulate system, we “tile” each cell with a particle that takes a certain fraction ϕ_f of the cell. We numerically demonstrate hyperuniformity of the resulting systems in terms of local volume-fraction variances.

B3: Zheng Ma, Princeton University
Coauthor: Salvatore Torquato
Precise algorithms to compute surface correlation functions of two-phase heterogeneous media and their applications

Abstract: The quantitative characterization of the microstructure of random media in d-dimensional Euclidean space is of great importance. In particular, the study of different types of two-point correlation functions has proved fruitful not only with respect to inferring effective properties but also for microstructure reconstructions. Specically, the surface-surface and surface-void correlation functions (obtainable from radiation scattering experiments) contain crucial interfacial information that determine transport properties of the media (e.g., the mean survival time and fluid permeability) and complement the information of the conventional two-point correlation function. However, current technical difficulty involved in sampling surface correlation functions has been a stumbling block in their widespread use. We first show that the small-r behaviors of these functions are linked to the mean curvature of the system. Then we demonstrate that one can reduce the computational complexity of the problem without sacrificing accuracy by extracting the necessary interfacial information from a cut of the d-dimensional statistically homogeneous and isotropic system with a m-dimensional subspace. Accordingly, we devise algorithms based on this idea and test them for two-phase media in continuous and discrete spaces. Specifically for the exact benchmark model of overlapping spheres, we find excellent agreement between numerical and exact results. We compute surface correlation functions and corresponding surface-area variances for a variety of systems, including overlapping spheres, hard spheres in equilibrium, decorated ``stealthy'' patterns, as well as snapshots of evolving pattern formation processes. It is demonstrated that the precise determination of surface correlation functions provides a powerful means to characterize a wide class of complex multiphase microstructures.

B4: Jasen Scaramazza
Coauthors: Joel Lebowitz, Abhishek Dhar, Aritra Kundu
Unexpected transport properties of the classical Toda chain with harmonic pinning

Abstract: We investigate, via numerical simulation, heat transport in the nonequilibrium stationary state (NESS) of the 1D classical Toda chain with an additional pinning potential, which destroys momentum conservation. The NESS is produced by coupling the system, via Langevin dynamics, to two reservoirs at different temperatures. To our surprise, we find that when the pinning is harmonic, the heat transport appears to be superdiffusive, perhaps even ballistic. This behavior is expected for an integrable model, but not in the present model where integrability is broken and momentum conservation violated. This work is ongoing in collaboration with Joel Lebowitz, Abhishek Dhar and Aritra Kundu.