121st STATISTICAL MECHANICS CONFERENCE SHORT TALK SCHEDULE

SESSION A

A1: Pavel Dubovski, Stevens Institute of Technology
A result on mass conservation for coagulation-fragmentation equation.
Coauthors : C.Moakler
Abstract : For the coagulation-fragmentation Smoluchowski equation, we prove both computationally and analytically that for certain typical kernels (rates) of coagulation and fragmentation the mass conservation law is broken but the mass does not decay to zero.

A2: Peter Townsend, Rutgers University
Statistical mechanics and the helium-3 surface spin echo experiment
Abstract : Modelling the diffusion of mobile chemical species adsorbed on solid surfaces is a classic application of statistical mechanical methods. Correlation functions in space and time provide a powerful statistical summary of the diffusion process, and can be compared to the results of spectroscopic scattering experiments to acquire a detailed physical understanding of real adsorption systems. In particular, the helium-3 surface spin echo experiment allows surface dynamics to be probed on time scales in a window from approximately one picosecond to one nanosecond, at atomic length scales. I will discuss two ways in which such measurements are senstive to the details of the dissipative coupling between adsorbates and the surface. The two examples are linked by the theme of memory effects.

A3: Eugene Kolomeisky, University of Virginia
Steady flows, nonlinear gravitostatic waves and Zeldovich pancakes in a Newtonian gas
Abstract: We show that equations of Newtonian hydrodynamics and gravity describing one-dimensional steady gas flow possess nonlinear periodic solutions. In the case of a zero-pressure gas the solution exhibits hydrodynamic similarity and is universal: it is a lattice of integrable density singularities coinciding with maxima of the gravitational potential. With finite pressure effects included, there exists critical matter density that separates two regimes of behavior. If the average density is below the critical, the solution is a density wave which is in phase with the wave of the gravitational potential. If the average density is above the critical, the waves of the density and potential are out of phase. Similar conclusions apply to traveling gravitostatic waves. Specifically, for subsonic motion the wave is made out of two out of phase oscillations of matter density and gravitational potential. If the motion is supersonic, the density-potential oscillations in the wave are in phase.

A4: Jeremiah Birrell, University of Massachusetts Amherts
Coauthors: Luc Rey-Bellet
Abstract: I will discuss a method for obtaining concentration inequalities and confidence intervals for several classes of hypo-coercive stochastic systems, including underdamped Langevin and several classis of Markov Hain Monte Carlo samplers.

A5: Gregory Dignon, Lehigh University
Relationship between single chain properties and phase separation of intrinsically disordered proteins
Coauthors: Wenwei Zheng, Young C. Kim, Jeetain Mittal
Abstract: Liquid-liquid phase separation of intrinsically disordered proteins has been identified as an important process within biology. It allows for the compartmentalization of biomolecules for various functions requiring localization and concentration of particular biomolecules. Phase separated protein assemblies also provide a promising strategy for applications in drug delivery and biomaterials. Coarse-grained simulations can aid in the study of liquid-like assemblies of disordered proteins at the sequence level, directly representing the protein sequence as well as giving access to sufficient time and length scales to directly interrogate phase coexistence. Here I describe the important contributions our group has made in the field of biomolecular phase separation using amino acid resolution coarse-grained simulations.

A6: Yu-Chen Cheng, University of Washington

Coauthors : Hong Qian

Abstract : A cardiovascular system can be simply modeled by three components and three connections. The three components: the heart, the artery, and the vein - all can be treated as elastic tubes. Each elastic tube is characterized by linear elasticity with its natural volume. The active cardiac contraction element is represented by a change of elasticity for the heart, which is an emergent phenomenon: a collective behaviors of the release of calcium from cardiac muscles triggered by an spread of action potential for a short period of time. High elasticity represents that the heart is in the state of contraction; Low elasticity represents that the heart is in the state of relaxation. Three connections are the inflow valve, the outflow valve and microvessels, respectively. The inflow valve only allows one-way flow from the vein to the heart; The outflow valve only allows one-way flow from the heart to the artery; Microvessles allow two-way flow bewteen the artery and the vein with equivalent resistances. By this naive model, we are able to describe continuous blood flows generated by alternations of the systolic phase (heart contraction) and the diastolic phase (heart relaxation). In order to build a solid concept of {\em macroscopic entropy production} in the process, we do a stochastic analysis of a couple diffusion model for our toy physical descriptions for the cardiovascular system.

A7: Chen Yong-Cong, Shanghai University

Title：Large scale kinetic modeling of metabolic networks.

While the biochemistry of metabolism in many organisms is well studied, details of the metabolic dynamics are not fully explored yet. Acquiring adequate in vivo kinetic parameters experimentally has always been an obstacle. Unless the parameters of a vast number of enzyme-catalyzed reactions happened to fall into very special ranges, a kinetic model for a large metabolic network would fail to reach a steady state. In this talk we show that a stable metabolic network can be systematically established via a biologically motivated regulatory process. The regulation is constructed in terms of a potential landscape description of stochastic and nongradient systems. The constructed process draws enzymatic parameters towards stable metabolism by reducing the change in the Lyapunov function tied to the stochastic fluctuations. Our approach allows further constraints such as thermodynamics and optimal balance of efficiency vs viability.

A8: Ang Gao, Massachusetts Institute of Technology

Evolution of weak cooperative interactions for biological specificity

Coauthors: Krishna Shrinivas; Paul Lepeudry; Hiroshi I Suzuki; Phillip Sharp; Arup K Chakraborty

Abstract: A hallmark of biological systems is that particular functions and outcomes are realized in specific contexts, such as when particular signals are received. One mechanism for mediating specificity is described by Fisher’s “lock and key” metaphor, exemplified by enzymes that bind selectively to a particular substrate via specific finely tuned interactions. Another mechanism, more prevalent in multicellular organisms, relies on multivalent weak cooperative interactions. Its importance has recently been illustrated by the recognition that liquid-liquid phase transitions underlie the formation of membraneless condensates that perform specific cellular functions. Based on computer simulations of an evolutionary model, we report that the latter mechanism likely became evolutionarily prominent when a large number of tasks had to be performed specifically for organisms to function properly. We find that the emergence of weak cooperative interactions for mediating specificity results in organisms that can evolve to accomplish new tasks with fewer, and likely less lethal, mutations. We argue that this makes the system more capable of undergoing evolutionary changes robustly, and thus this mechanism has been repeatedly positively selected in increasingly complex organisms. Specificity mediated by weak cooperative interactions results in some useful cross-reactivity for related tasks, but at the same time increases susceptibility to mis-regulation that might lead to pathologies.

A9: Andreas Mayer, Princeton University

A statistical ensemble approach to immune discrimination

Coauthors: Q Marcou, BD Greenbaum, W Bialek

Abstract: The immune system needs to distinguish molecular signatures of pathogens from those found in the organisms' own proteins. A naive, but universal way to discriminate is to whitelist everything that should not elicit a reaction. Can the immune system do better? To begin to answer this question we characterize the self and pathogen proteomes as statistical ensembles. Probabilistic models reveal how both universal and phyla-specific constraints on protein evolution shape the statistics of the proteomes. The models furthermore allow us to quantify to what extent the ensembles differ systematically. We analyze whether and how these differences might be used for efficient immune defense. Finally, we compare predictions to what is known about epitopes recognized by the immune system.

A10: Nigel Goldenfeld, University of Illinois at Urbana-Champaign
Topological scaling laws and the statistical mechanics of evolutionary trees
Coauthors: Chi Xue, Zhiru Liu
Abstract: For the last 3.8 billion years, the large-scale structure of evolution has followed a pattern of speciation that can be described by branching trees. Recent work, especially on bacterial sequences, has established that despite their apparent complexity, these so-called phylogenetic or evolutionary trees exhibit two unexplained broad structural features which are consistent across evolutionary time. The first is that phylogenetic trees exhibit scale-invariant topology, which quantifies the fact that their branching lies in between the two extreme cases of balanced binary trees and maximally unbalanced ones. The second is that the backbones of phylogenetic trees exhibit bursts of diversification on all timescales. I present a coarse-grained statistical mechanics model of ecological niche construction coupled to a simple model of speciation, and use renormalization group arguments to show that the statistical scaling properties of the resultant phylogenetic trees recapitulate both the scale-invariant topology and the bursty pattern of diversification in time. These results show in principle how dynamical scaling laws of phylogenetic trees on long time-scales may emerge from generic aspects of the interplay between ecological and evolutionary processes.

SESSION B

B1: Sungchul Ji, Ernest Mario School of Pharmacy, Rutgers University
Quantum Genetics': The Quantization of Genes
Abstract : Genes can be defined as any segments of DNA, n-nucleotide long (where n = 1, 2, 3, ..., 10^9), that participate in transmitting genetic information from one cell generation to the next [1]. Thus defined, the whole DNA molecule can be viewed as a gene, since it is replicated from one cell generation to the next. The purpose of this presentation is to discuss the emerging new discipline in genetics that is based on both the quantitative (i.e., copy number variation) and the qualitative (i.e., nucleotide sequence variation) aspects of genes consistent with the quantity-quality complementarity which may be related to the particle-wave duality or complementarity [2]. The newly emerging discipline is characterized by the quantization of genetic information (in the form of copy number variations [3]) in analogy to the emergence of quantum mechanics (QM) following the quantization of energy (or action) in 1900 and hence is here referred to as “quantum genetics (QG)”. One possible mechanism of action of copy numbers on gene properties involves the mass-dependent vibrational frequencies of genes, since f = (k/m)^-2, where f is the frequency, m is the gene mass, and k is the spring constant of chemical bonds within a gene, between two or more genes, or between genes and their extracellular environments. Recent evidence indicates that the biology of DNA, RNA and proteins is dependent on the vibrational motions of these biopolymers [4, 5, 6]. An advantage of the vibrational approach to understanding biopolymer functions is the natural way that different regions within a biopolymer (or between two or more biopolymers, or even between genes and their extracellular environments) can communicate or couple through the mechanism of resonance [5, 6]. The transition from classical mechanics to QM took about a quarter of a century, from 1900 to 1925. The transition from classical genetics to quantum genetics may take much longer, perhaps at least one century (?). References: [1] Ji, S. (2012). What Is a Gene? In: Molecular Theory of the Living Cell: Concepts, Molecular Mechanisms, and Biomedical Applications. Springer, New York. Section 11.2. [2] Ji, S. (2015). Planckian distributions in molecular machines, living cells, and brains: The wave-particle duality in biomedical sciences. In: Proceedings of the International Conference on Biology and Biomedical Engineering, Vienna, March 15-17, 2015. Pp. 115-137. PDF at http://www.conformon.net/wp-content/uploads/2016/09/PDE_Vienna_2015.pdf [3] Wain, L. V., Armor, J. A., and Tobin, M. D. (2009). Genomic copy number variation, human health, and disease. Lancet 374: 340-350. [4] Ji, S. (2019). The Cell Language Theory: Connecting Mind and Matter. World Scientific Publishing, New Jersey. [5] Ji, S. (2018). RASER Model of Single-Molecule Enzyme Catalysis and Its Application to the Ribosome Structure and Function. Arch. Mol. Med. Genet. 1(1): 31-39. [6] Petoukhov S.V. (2017). Genetic coding and united-hypercomplex systems in the models of algebraic biology. Biosystems 158: 31-46.

B2: Alexander Siegenfeld, Massachusetts Institute of Technology
Negative Representation and Instability in Democratic Elections
Coauthors: Yaneer Bar-Yam
Abstract: Motivated by the troubling rise of political extremism and instability throughout the democratic world, we present a novel mathematical characterization of the nature of political representation in democratic elections. We

define the concepts of negative representation, in which a shift in electorate opinions produces a shift in the election outcome in the opposite direction, and electoral instability, in which an arbitrarily small change in opinion causes a large change in election outcome. Under very general conditions, we prove that unstable elections necessarily contain negatively represented opinions. Furthermore, increasing polarization of the electorate can drive elections through a transition from a stable to an unstable regime, analogous to the phase transition by which some materials become ferromagnetic below their critical temperatures. In this unstable regime, a large fraction of political opinions are negatively represented. Empirical data suggest that United States presidential elections underwent such a phase transition in the 1970s and have since become increasingly unstable.

B3: Anatolij Prykarpatski, Institute of Mathematics at the Cracov University of Technology, Cracow, Poland
The current algebra representations of quantum many-particle Schrödinger type Hamiltonian models, their factorized structure and integrability
Coauthors: Denis Blackmore and Dominik Prorok
Abstract: There is developed the G. Goldin's algebraic factorization scheme of constructing density operator and functional representations for the canonical local quantum current algebra and its application to quantum Hamiltonian and symmetry operators reconstruction in case of quantum integrable spatially many- and one-dimensional dynamical systems. The quantum generalized oscillatory, Calogero-Sutherland, Coulomb type and Nonlinear Schrödinger models of spin-less bose-particles are analyzed in details.

B4: Suhov Yuri, Math Dept, Penn State University
Hard-core configurations in a plane and a 2D lattice
Coauthors : A. Mazel, I. Stuhl
Abstract : The hard-core model attracted interest at an early stage of the progress in the rigorous Statistical Mechanics; its popularity increased after recent successes in studying dense-packing configurations of hard spheres in ${\mathbb R}^d$, for $d=2,3,8,24$ and in view of new applications, in particular in Computer Science and Biology. We focus on two problems: (i) specification of periodic configurations of the maximum density which cannot be `improved' by a local change (periodic ground states, PGSs for short), and (ii) identification of the dominant PGSs generating extreme Gibbs/DLR measures for large values of fugacity by means of the Pirogov-Sinai theory. This presentation will be limited to the 2D case where hard-core particles are represented by disks of a given diameter D (the hard-core exclusion distance measured in the Euclidean metric).

B5: Izabella Stuhl, Penn State
Hard-core model in 2D: high-density ground states and Gibbs measures
Coauthors: Alik Mazel, Izabella Stuhl*, Yuri Suhov
Abstract: We will discuss ground states and Gibbs measures for the hard-core model at a high-density with arbitrary exclusion distances on a unit triangular/square lattice.

B6: Nikolai Bogolyubov, Mathematical Institute Steclov Moscow Russia
Model Systems with repulsive interactions in statistical mechanics**.**
Abstract : A general class of model systems with separable repulsive interactions is studied. Conditions for the asymptotic exactness of the approximating Hamiltonian approach are given and some applications are discussed

B7: Mukhayo Rasulova, Institute of Nuclear Physics Academy of Sciences Republic of Uzbekistan
Application of solution of the quantum kinetic equations for information technology.
Abstract: The existence of unique solution, in terms of initial data of the hierarchy of quantum kinetic equations with delta potential and application of kinetic equation for information technology, has been proven. The proof is based on the non-relativistic quantum mechanics and application of semi group theory methods

B8: Mohamed El Hedi Bahri, Princeton University
Influence of Thermal Fluctuations on the Mechanical Properties of 2D Anisotropic Materials
Coauthors: Andrej Košmrlj
Abstract: We present the field theory of a general elastically anisotropic 2-dimensional sheet, which is permitted to fluctuate out of plane. The field theory for isotropically elastic sheets of infinite size was developed in the 80s via the Renormalization Group in which a non-trivial fixed point was found. The values of universal exponents associated with this “isotropic” fixed point indicate a divergence of bending rigidity with the system size, while the Young's modulus

and other in-plane elastic moduli decay toward zero. By generalizing the field theory for anisotropic materials, we uncovered that the isotropic fixed point is unstable to perturbations that correspond to materials with the orthorhombic symmetry, which under RG transformation flow towards a new fixed point. The universal exponents for this “orthorhombic” fixed point are different from the ones for the isotropic materials. Furthermore, we observe that elastic moduli along one principal axis scale with a different exponent than the corresponding ones along the orthogonal axis, and therefore the anisotropy gets amplified with increasing system size. Finally, we systematically analyzed the RG flow of elastic constants for materials that belong to all 17 distinct crystallographic space groups and we found that they flow either to the “isotropic” or to the “orthorhombic” fixed point. From this we deduce that thermal fluctuations generate an effective mirror symmetry for elastic properties, which may have not been present microscopically, such as for the monoclinic lattice.

B9: Jaeuk Kim, Princeton University
Tessellation-based methodology to construct perfectly hyperuniform disordered packings [1,2].
Coauthors : Salvatore Torquato
Abstract : Disordered hyperuniform packings (or dispersions) are unusual amorphous states of two-phase materials that are characterized by an anomalous suppression of volume-fraction fluctuations at infinitely long-wavelengths, compared to ordinary disordered materials. While there has been growing interest in disordered hyperuniform materials, a major obstacle has been an inability to produce large samples that are perfectly hyperuniform due to practical limitations of conventional numerical and experimental methods. To overcome these limitations, we introduce a general theoretical methodology to construct perfectly hyperuniform packings in d-dimensional Euclidean space. Specifically, beginning with an initial general tessellation of space by disjoint cells that meets a “bounded-cell” condition, hard particles are placed inside each cell such that the volume fraction of this cell occupied with these particles becomes identical to the global packing fraction. We prove that the constructed packings with a polydispersity in size are perfectly hyperuniform in the infinite-sample-size limit. We numerically implement this procedure to two distinct and important types of initial tessellations: Voronoi as well as sphere tessellations. Beginning with Voronoi tessellations, we show that our algorithm can remarkably convert extremely large nonhyperuniform packings into hyperuniform ones in two and three dimensions. Application to sphere tessellations establishes the hyperuniformity of the classical Hashin-Shtrikman multiscale coated-spheres structures that possess optimal effective transport and elastic properties. [1] J. Kim and S. Torquato, “New tessellation-based procedure to design perfectly hyperuniform disordered dispersions for materials discovery,” Acta Mater. 168, 143-151, (2019) [2] J. Kim and S. Torquato, “Methodology to Construct Large Realizations of Perfectly Hyperuniform Disordered packings,” arXiv preprint: 1901.10006 (2019).

B10: Raman Ganti, Massachusetts Institute of technology
n/a
Coauthors :Arup K. Chakraborty
Abstract : A T lymphocyte's capacity to discriminate between foreign and self antigens is a remarkable feat of the immune system. Only a few agonists in a sea of noise can reliably activate the T cell's downstream signaling cascade. Kinetic proofreading proposes that discriminatory capability depends on a single parameter, the lifetime of T cell receptor-ligand bonds. We show via an information theoretic measure of discrimination, channel capacity, that the T cell has developed clever mechanisms to separate a small amount of signal from large external noise. By combining known biological details of T cell signal transduction with kinetic proofreading rules, we show that channel capacity directly quantifies discrimination for all possible self ligand concentrations, which is preferable to previous indirect measures. As a consequence, we can clearly explain the role of kinetic bottlenecks and feedback loops in T cell signal processing.

SESSION C

C1: Jeffrey Thompson, the University of Texas at Austin
A lower bound on the neutral grand canonical partition function of a charge-symmetric system
Coauthors: Isaac C. Sanchez (UT Austin)
Abstract: We adapt to the neutral grand canonical ensemble a lower bound obtained by Kennedy (J. Stat. Phys. 28:633, 1982) on the ordinary grand partition function of a charge-symmetric system. The neutral ensemble permits us to consider interaction potentials which are only conditionally positive definite, for instance, the logarithmic potential $-\log(1+|x-y|)$. The correlation length which appears in our lower bound increases with decreasing volume; it converges to the ordinary grand canonical value in the infinite-volume limit. This volume dependence is tied to an effect termed "canonical suppression" in high energy nuclear physics, whereby the density of a ideal gas of charged particles in the grand canonical ensemble is suppressed by the restriction to charge-neutral configurations.

C2: Marc Potters, Capital Fund Management (Paris)
Signal and noise in large sample covariance matrices
Coauthors: Jean-Philippe Bouchaud, Joel Bun
Abstract: Large sample covariance matrices (SCM) are not the best estimates of true covariance's. Using tools from random matrix theory (RMT) and free probability one can compute the eigenvalue spectrum of the SCM from independent or even auto-correlated samples. One can also compute the optimal estimator of true covariance from sample data under a natural hypothesis of absence of prior knowledge about eigenvectors. This estimator can be expressed in RMT language but is easier to understand in the optimization/validation (O/V) framework used in machine learning. I speculate that the link between the RMT and O/V frameworks can help us distinguish between signal and noise in very complex noisy data sets such as neural recording data. References: Bun, Bouchaud and Potters, Physics Reports 666 (2017), forthcoming book by Potters and Bouchaud, Cambridge (2020).

C3: Guillaume Dubach, Courant Institute
Moments of the characteristic polynomial of Ginibre matrices
Coauthors: P. Bourgade, L. Hartung
Abstract: The proof of convergence to Gaussian Multiplicative Chaos for the characteristic polynomial of the complex Ginibre ensemble involves a precise asymptotical formula for its moments. I will present this formula and comment upon its proof and significance.

C4: Peter Nandori, University of Maryland
Global observables for random walks: law of large numbers
Coauthors: Dmitry Dolgopyat, Marco Lenci
Abstract: We consider the sums $T_N = \sum_1^N F(S_n)$, where S_n is a random walk on Z^d and $F : Z^d \to R$ is a global observable, that is, a bounded function which admits an average value when averaged over large cubes. We show that TN always satisfies the weak Law of Large Numbers but the strong law fails in general. Under additional regularity assumptions on F, we obtain the Strong Law of Large Numbers and estimate the rate of convergence. The growth exponents which we obtain turn out to be optimal in two special cases: for quasiperiodic observables and for random walks in random scenery.