

118th STATISTICAL MECHANICS CONFERENCE

SHORT TALK SCHEDULE

SESSION A

A1: Matthew Marko, US Navy/Rutgers University

The Temperature Dependence on Intermolecular Potential Energy in the Design of a Supercritical Stirling Cycle Heat Engine

Abstract: The Stirling thermodynamic heat engine cycle is modified, where instead of an ideal gas, a real, supercritical, monatomic working fluid subjected to intermolecular attractive forces is used. The potential energy of real gases is redefined to show it decreasing with temperature as a result of the attractive Keesom forces, which are temperature dependent. This new definition of potential energy is used to thermodynamically design a Stirling cycle heat engine with supercritical xenon gas, and an engine efficiency that exceeds the Carnot efficiency is demonstrated. The change in internal energy predicted is compared to experimental measurements of condensing steam, xenon, argon, krypton, nitrogen, methane, ethane, propane, normal butane, and iso-butane, and the close match validates this new definition of temperature-dependent real gas potential energy, as well as the thermodynamic feasibility of the modified supercritical Stirling cycle heat engine. <https://arxiv.org/abs/1709.06852>

A2: Duyu Chen, Princeton University

Coauthors: Michael A. Klatt, Jakov Lovrić, Duyu Chen, Sebastian C. Kapfer, Fabian M. Schaller, Philipp W. A. Schönhöfer, Bruce S. Gardiner, Ana-Sunčana Smith, Salvatore Torquato, and Gerd E. Schröder-Turk
Universal hidden order in amorphous cellular geometries

Abstract: Starting from an amorphous partitioning of space into cells, we iteratively optimize the “centrality” of the cells, minimizing the so-called Quantizer energy. The energy landscape is replete with local minima to which the system converges despite the existence of lower-energy crystalline configurations. Irrespective of the level and type of disorder in the initial configurations, the tessellations converge to the same amorphous state, as measured by the same structure factor and energy distributions. The final disordered configurations exhibit an anomalous suppression of long-wavelength density fluctuations, known as hyperuniformity. For systems related to the Quantizer problem, such as self-assembled copolymeric phases, our findings suggest the possibility of stable disordered hyperuniform phases.

A3: Alexander Khaneles, AT&T

Does the blackbody radiation spectrum suggest an intrinsic structure of photons?

Abstract: Photons are considered to be elementary bosons in the Standard Model. An assumption that photons are not elementary particles is assessed from an outlook of equilibrium statistical mechanics with insights from computer simulation.

A4: Ronald Fisch, Retired

Scaling Beyond the Imry-Ma length in the 3D Random-Field XY Model

Abstract: TBA

A5 1: Jaeuk Kim, Princeton University

Effect of phonon excitations on the hyperuniformity of crystals

Abstract: Hyperuniformity is the state of matters where density fluctuations on large length scales are significantly suppressed [i.e., structure factors become zero as wavenumber approaches to zero], relative to typical disordered systems. Hyperuniform systems include all crystals, quasicrystals, and some exotic disordered systems, and especially disordered hyperuniform systems are gathering attention due to their

unusual properties. However, any compressible one-component system in thermal equilibrium cannot be hyperuniform at positive temperatures due to thermal excitations, which follows from the fluctuation-compressibility relation [1]. To directly demonstrate that the nonhyperuniformity of thermalized systems is attributed to thermally excited longitudinal acoustic modes, we studied cubic crystals in the classical harmonic regime. Without using the Debye-Waller factor, we derive the leading order approximation of structure factors of thermalized cubic crystals, which corresponds to one-phonon scattering. Our result is consistent with computer simulations at low temperatures as well as the compressibility relation. References [1] S. Torquato, G. Zhang, and F. Stillinger, PRX 5, 021020 (2015)

A5: Gustavo R. Perez-Lemus, Universidad Nacional Autonoma de Mexico

Coauthors : Quintana-H. Jacqueline

Liquid crystal phases in soft repulsive organic cages models

Abstract : Organic cages molecules are a relative novel type of porous material that presents polymorphism in solid state and it has been used in many applications given their porosity and structure. We propose a soft repulsive model of this type of molecules and use molecular dynamics simulations to study their phase diagram. The results show the presence of liquid-crystalline phases that depends on the porosity and intrinsic symmetry of the molecules.

Reservation Request : I do not wish to share a room

A6: Lee Jinwoo, Kwangwoon University

Coauthors: Hajime Tanaka (University of Tokyo)

Viewpoint dependence of thermodynamic direction of time

Abstract: Bio-molecules are active agents in that they consume energy to do work upon an object, and here we are interested in the situation where an active agent (e.g. a helicase molecule) is working upon an object (e.g. DNA) in a heat bath. If one defines viewpoint as the location of an agent which applies work upon an object, the formula describing the first law of thermodynamics ($W = \Delta E + Q$, where W is applied work upon a system and Δ is the change in the internal energy of the system and Q is heat dissipated into the environment) can be characterized as a system-external viewpoint since the degrees of freedom of the work agent is excluded from those of the system in general. If one considers a composite system composed of the agent and object, no thermodynamic work is involved since we have $W = 0 = \Delta E + Q$. Here we introduce a new framework that can be characterized as a system-internal viewpoint in that it considers the active agent as parts of the system while applying thermodynamic work upon the object. To analyze this situation, we introduce Ψ which is a non-equilibrium counterpart of the equilibrium free energy without requiring a local equilibrium assumption. We found that Ψ tends to be maximized in the system-internal viewpoint contrary to the conventional case of system-external viewpoint where Ψ tends to be minimized. Reference: Lee Jinwoo and Hajime Tanaka, Physical description of nature from a system-internal viewpoint, arXiv: 1705.01234 (2017)

A7: Eugene Kolomeisky, University of Virginia

Kelvin-Mach wake in a two-dimensional Fermi sea

Abstract: The dispersion law of plasma oscillations of a two-dimensional electron gas in the hydrodynamic approximation interpolates between the square root of the wave vector " q " dependence for " q " small to the linear one for " q " large. As a consequence, downstream of a charged impurity in the presence of a uniform supersonic current flow, a peculiar wake pattern of induced charge density and potential is formed whose geometry is controlled by the Mach number. Specifically, for Mach numbers below the square root of 2 the wake consists of transverse wavefronts confined within a sector whose angle is given by the classic Mach condition. An additional wake of larger opening angle outside the Mach sector that resembles the Kelvin ship wake and consists of both transverse and diverging wavefronts is found for Mach numbers exceeding the square root of 2.

SESSION B

B1': Sungchul Ji – Rutgers University

Planck-Shannon space: A novel quantitative method to identify functionally related metabolic pathways (or Planckons) in cell biology

Abstract: In 2008, at the 100th meeting of this Conference [1, 2], I reported the derivation of Equation (1) referred to as the Planckian Distribution Equation (PDE) from the blackbody radiation equation discovered by M. Planck in 1900 by replacing its universal constants and temperature with free parameters, A, B and C:

$$y = A/(x+B)^5/(eC/(x + B) - 1) \quad (1)$$

PDE has been found to fit almost all long-tailed histograms we have analyzed so far that have been reported in the fields of atomic physics, molecular biology, cell biology, neurophysiology, psychology, glottometrics (also called quantitative linguistics), econometrics, cosmology [3-6], 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]. There are two ways of quantifying the information content of PDE:

Plankian information of the first kind: $IPF = \log_2 [AUC (PDE)/AUC (GLE)] \quad (2)$

Plankian information of the second kind: $IPS = -\log_2 [(\mu - mode)/(\sigma)] \quad (3)$

where AUC = Area Under the Curve; GLE = Gaussian-Like Equation whose rising portion approximate closely the rising portion of PDE, and μ and σ are, respectively, the mean and the standard deviation of the data set that fits PDE. In addition PDE allows us to calculate the associated Shannon entropy as

$$H = -\sum_i (\pi_i \log_2 \pi_i) \quad (4)$$

where \sum_i is the sum over i from 1 to n , the number of data points, and π_i is the probability of the occurrence of the i th data point.

We have analyzed the mRNA level data of the arbitrarily selected 10 metabolic pathways measured from human breast tissues using microarrays [8]. Each metabolic pathway was encoded by 30 to 175 genes or ORF (open reading frames): cell cycle 72; cell wall biogenesis, 53; chromatin structures, 44; cytoskeletons, 71; DNA repair, 32; rRNA processing 37; nuclear protein targeting, 43; protein synthesis, 156; transport, 129; and transcription, 175. These data sets all fitted PDE, thus generating 10 pairs of the IPF and H values. [Since any physicochemical processes generating long-tailed histograms fitting PDE are defined as “Planckian processes” [3-5] (or Planckons, for brevity), and since the mRNA levels encoded by many metabolic pathways examined so far fit PDE, we can identify the physicochemical processes underlying metabolic pathways as “Planckons”, a neologism introduced here for the first time.] When these 10 pairs of numbers were plotted in the so-called “Planck-Shannon space (PSS)”, a linear correlation was found with the R^2 value of 0.686. However, when similar sets of the mRNA levels that have no known metabolic functions were plotted on the PSS, no correlation was found, the R^2 value being 0.213, far less than 0.7, the minimum threshold for a significant correlation. Hence, we can conclude that the Planck-Shannon plot can be used to identify functionally related set of metabolic pathways or Planckons. Based on the postulate of the isomorphism between cell and human languages [9-11] that cells use a molecular language, we can identify mRNA molecules as cell-linguistic words (i.e., the components of Planckons), metabolic pathways as cell-linguistic sentences (i.e., Planckon), and the functionally related sets of metabolic pathways (or systems of Planckons) as cell-linguistic texts. Therefore, it seems reasonable to conclude that the Planck-Shannon plots devised in 2017 based on PDE can be used to identify molecular sentences and molecular texts based on dynamic mRNA level data that was predicted to exist in the living cell by the cell language theory proposed in 1997 [9-11].

References:

- [1] 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 Mechanics Conference, December 13-16, Rutgers University, Piscataway, N.J.
- [2] Ji, S. (2012). Molecular Theory of the Living Cell: Concepts, Molecular Mechanisms, and Biomedical Applications. Springer, New York. Pp 343-368.
- [3] 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

[4] Ji, S. (2015). PLANCKIAN INFORMATION (IP): A NEW MEASURE OF ORDER IN ATOMS, ENZYMES, CELLS, BRAINS, HUMAN SOCIETIES, AND THE COSMOS. In: Unified Field Mechanics: Natural Science beyond the Veil of Spacetime (Amoroso, R., Rowlands, P., and Kauffman, L. eds.), World Scientific, New Jersey, 2015, pp. 579-589. PDF at http://www.conformon.net/wp-content/uploads/2016/09/PDE_Vigier9.pdf

[5] Ji, S. (2016). WAVE-PARTICLE DUALITY IN PHYSICS AND BIOMEDICAL SCIENCES. Symmetry: Science and Culture 27 (2): 99-127 (2016).

PDF at http://www.conformon.net/wp-content/uploads/2016/09/PDE_SymmetryFestival_2016.pdf

[6] Ji, S. (2017). The Cell Language Theory: Connecting Mind and Matter. World Scientific Publications, New Jersey. Chapter 8.

[7] Unpublished observations made in collaboration with Pedro Marijuan of Zaragoza, Spain.

[8] Perou, C. M., Sorlie, T., Eisen, M. B., et al. (2000). Molecular portraits of human breast Tumors. Nature 406(6797):747-52.

[9] Ji, S. (1997). Isomorphism between cell and human languages: molecular biological, bioinformatic and linguistic implications. BioSystems 44: 17-39.

PDF at <http://www.conformon.net/wp-content/uploads/2012/05/Isomorphism1.pdf>

[10] Ji, S. (1999). The Linguistics of DNA: Words, Sentences, Grammar, Phonetics, and Semantics. Ann. N. Y. Acad. Sci. 870:411-417.

[11] Ji, S. (2017). The Cell Language Theory; Connecting Mind and Matter. World Scientific Publications. New Jersey. **B1: Bayram Deviren, Nevsehir Haci Bektas Veli University**

Coauthors: Seyma Akkaya Deviren

Magnetic properties of mixed spin-1 and spin-3/2 Ising nanoparticles with core-shell structure

Abstract: The magnetic properties of mixed spin-1 and spin-3/2 Ising nanoparticles with core/shell structure are studied by using the effective-field theory with correlations. We investigate the thermal variations of the core, shell and total magnetizations and the Q-, R-, P-, S-, N- and L-types of compensation behavior in Néel classification nomenclature exists in the system. The effects of the crystal-field, core and shell interactions and interface coupling, on the phase diagrams are investigated in detail and the obtained phase diagrams are presented in three different planes. The system exhibits both second- and first-order phase transitions besides tricritical point, double critical end point, triple point and critical end point depending on the appropriate values of the interaction parameters. The system strongly affected by the surface situations and some characteristic phenomena are found depending on the ratio of the physical parameters in the surface shell and the core. This work is supported by the Scientific Project Fund of Nevsehir University Haci Bektas Veli University under the project number: NEÜLÜP16F3.

B2: Sergey Belan, Massachusetts Institute of Technology

Bernoulli experiment under restart

Abstract: Recently noticed ability of restart to reduce the expected completion time of first-passage processes allows appealing opportunities for performance improvement in a variety of settings. However, complex stochastic processes often exhibit several possible scenarios of completion which are not equally desirable in terms of efficiency. I will demonstrate that restart may have profound consequences on the splitting probabilities of a Bernoulli-like first-passage process, i.e. of a process which can end with one of two outcomes. Particularly intriguing in this respect is the class of problems where a carefully adjusted restart mechanism maximizes probability that the process will complete in a desired way. The universal aspects of this kind of optimal behaviour can be revealed by applying the general approach recently proposed for the problem of first-passage under restart.

B3: Soon Hoe Lim, The University of Arizona

Coauthors: Jan Wehr, Aniello Lampo, Miguel Ángel García-March, Maciej Lewenstein

On the Small Mass Limit of Quantum Brownian Motion with Inhomogeneous Damping and Diffusion

Abstract: In this short talk, I will outline our recent work on the small mass limit (or the Smoluchowski-Kramers limit) of a class of quantum Brownian motions with inhomogeneous damping and diffusion. For Ohmic bath spectral density with a Lorentz-Drude cutoff, we derive the Heisenberg-Langevin equations for the particle's observables using a quantum stochastic calculus approach. We consider an appropriately rescaled model and derive a limiting equation for the (slow) particle's position variable. We find that the limiting equation contains several drift correction terms, the quantum noise-induced drifts, including terms of purely quantum nature, with no classical counterparts

B4: Alex Solon, MIT

Coauthors: Yongjoo Baek, Xinpeng Xu, Nikolai Nikola, Yariv Kafri

Generic long-range interactions between passive bodies in an active fluid

Abstract: A single non-spherical body placed in an active fluid generates currents. We show that when two or more passive bodies are placed in an active fluid these currents lead to long-range interactions that can give rise to rich dynamics of the bodies. Using a multipole expansion we characterize their leading-order behaviors in terms of single-body properties.

B5¹: Maxim Zyskin– University of Nottingham

Carbon nanotube yarn and nanoenergetic material composites

Abstract: In recent experiments, it was shown that carbon nanotube yarns have unusual properties when expanded by nanoenergetic material explosion. I will describe modeling results to understand those experiments. Those materials have applications as actuators /artificial muscles

B5: Sheng Mao, Princeton University

Modeling multicomponent phase behavior inspired by membraneless compartmentalization in cells

Abstract: Recent evidence shows that intracellular phase separation can drive the formation of membraneless liquid-like droplets composed of protein RNA and other biomolecules. Gibbs rule suggests that the number of possible coexisting phases scales linearly with the number of components, which is on the order of hundreds in cells. However, in typical biological systems only a small number of phases are observed and they are often assembled in highly organized structures. To resolve this puzzle, we first employ Flory-Huggins theory to examine the global phase structure of many components, whose interaction energies are randomly drawn from a Gaussian distribution. We find that the typical number of coexisting phases is primarily determined by the composition and the mean strength of interaction. However, the enhanced variance of interaction increases the range of parameters, where small number of coexisting phases are observed. In order to see, how different phases evolve in time and arrange in space, we used the Cahn-Hilliard formalism. We investigate the nucleation and growth of domains as well as their relative packing for 3, 4, 5 and more components.

B6: David Pine, NYU

Coauthors: Lisa Tran, Abhrajit Laskar, & Ronjoy Adhikari

Configurations of a sedimenting chain from low to high Reynolds number

Abstract: The dynamics of a chain settling in a viscous fluid is governed by the balance of elastic, gravitational and hydrodynamic forces, of which only the latter depends on the fluid viscosity. Here we study the effect of varying viscosity, as quantified by the Reynolds number Re , on the settling dynamics of flexible chains of hollow metal beads of radius a . At low Re , linear conformations are unstable and chains settle in curved and writhing conformations but, surprisingly, at high Re they settle stably in linear horizontal conformations. We attribute this to a change in the strength and symmetry of the hydrodynamic forces as the inertial length a/Re becomes smaller than the chain length. Numerical simulations with Re -dependent hydrodynamic forces are in excellent agreement with experiment.