105th Statistical Mechanics Conference

SHORT TALK SCHEDULE

Session A

A1: H. Quan, University of Maryland, College Park
Coauthor(s): C. Jarzynski
Title: Maximum Efficiency of a Heat Engine Based on a Small System: Carnot Cycle at Nano Scale
Abstract: We study the maximum efficiency of a Carnot cycle heat engine based on a small system. It is found that irreversibility may arise due to the finiteness of the system. As a result there is a correction to the usual Carnot efficiency. We find a universal and simple expression for the maximum efficiency of a Carnot cycle heat engine based on a small system. This maximum efficiency approaches the usual Carnot efficiency when the dimension of the system increases to macroscopic size. Our study demonstrates the subtlety of thermodynamics in small systems.

A2: Speaker: M. Maghrebi, MIT
Coauthor: Y. Kantor and M. Kardar
Title: Correlations and critical exponents near the tip of a cone
Abstract: Correlation functions, for a Landau-Ginzburg model, are computed in the presence of a conical boundary, within mean-field and by expansion in d=4-\epsilon dimensions.
The critical exponent \eta varies continuously with the (half opening) angle \theta of the cone. We identify a new exponent governing the singular behavior of η as $\theta\to0$.

A3: Speaker: M. Novotny, Mississippi State University
Coauthor: S. Boettcher and C. Varghese
Title: Quantum Transport through Hanoi Networks
Abstract: We introduce a renormalization group (RG) method to calculate the quantum transmission of electrons within the tight-binding approximation. We apply the RG to transmission through two related Hanoi networks. HN3 has three bonds at every site, while HN5 adds additional bonds to make an average of five bonds per site. We observe band gaps for transmission through HN3 but not through HN5. A detailed scaling analysis near the edges of these bands are presented. See Phys. Rev. E, vol. 83, 041106 (2011).

A4: Speaker: B. Desinghu, Indiana University
Coauthor: P. Ortoleva
Title: Multiscale quantum simulations of nanoparticles: Role of effective mass and forces in electronic systems
Abstract: Electronic nanosystems involve the coupling of processes across a range of scales in space and time. Examples include quantum dots, superconducting or magnetic nanoparticles, molecular wires, and graphene nanoribbons. The number of electrons and strength of forces between them in these assemblies presents a challenge for traditional quantum computations. Recent theoretical results from deductive multiscale analysis (DMA) yield coarse-grained wave equations that capture the longer-scale quantum dynamics of these systems and suggest an efficient computational algorithm. We validate and demonstrate this multiscale quantum computational approach for metal nanoparticles. The Results illustrate the co-evolution of collective plasmonic dynamics with short-scale electron motion.

A5: Speaker: R. Fisch
Title: Subextensive singularity: The case of the 2D + -J Ising sping glass
Abstract: Recently, it has been shown by Thomas, Huse and Middleton[1] that the low temperature specific heat of the 2D Ising spin-glass behaves like 1/T3 in the thermodynamic limit. Earlier, it was shown[2] by the author that at fixed finite size the low temperature specific heat behaves like 1/T^{5.33 +- 0.12} for T < T_x, where T_x goes slowly to zero as the size of the sample goes to infinity. Thus one sees a different power law for the specific heat when taking the limit T -> 0 at fixed finite size, L x L, than one sees if the limit L -> infinity is taken before the limit T -> 0. This is a characteristic behavior of a subextensive singularity. The origin of this behavior appears to be the special behavior of zero-energy domain walls, which is caused by the topological long-range order[3] which exists in this model.
[1] C. Thomas, D. A. Huse and A. A. Middleton, arXiv:1103.1946v1
[2] R. Fisch, J. Stat. Phys. 128, 1113 (2007)
[3] C. Wang, J. Harrington and J. Preskill, Ann. Phys. (N.Y.) 303, 31 (2003)

A6: Speaker: G. Gulpinar, Dokuz Eylul University
Coauthor(s): E. Vatansever

Title: Temperature dependence of the complex susceptibility for a metamagnetic Ising model in the neighborhood of multicritical points.
Abstract: The kinetic equations of the order parameters of a metamagnetic system is derived by a method which combines the thermodynamics of irreversible processes and the equilibrium statistical mechanics of cooperative phenomena. By this method we described the time evolution of the order parameters by a set of linear equations of motion. After characterizing the time dependencies of the order parameters by two relaxation times, the steady state solution of the kinetic equations is obtained for the presence of a time-varying magnetic field. Then, the dynamic susceptibility ($\chi(\omega,T)= \chi'(\omega,T)+i\, \chi''(\omega,T)$) is derived as an function of field, frequency and temperature. Finally, we have represented the temperature dependence of magnetic dispersion and absorption factors in the neighborhood of multicritical points such as tricritical point, double critical point, and critical end point.

A7: Speaker: V. Golyk, Massachusetts Institute of Technology
Coauthors: Matthias Krüger and Mehran Kardar
Title: Heat radiation from thin cylindrical objects
Abstract: The heat radiated by objects whose sizes are comparable to thermal wavelength (in the micrometer range at room temperature) can be very different from the classical blackbody radiation described by Planck and Stefan-Boltzmann laws. Instead, methods based on scattering of electromagnetic waves can be used to explore the dependence on size, shape, as well as material properties. In particular, we explore the radiation from a heated long cylinder, which is polarized as allowed by symmetry. The degree and direction of polarization depends on the thickness and material properties of the cylinder. We briefly analyze different material classes (insulators, conductors and uniaxial materials).

A8: Speaker: H. Ge, Fudan University
Coauthor: H. Qian
Title: Local and global landscape confliction and its implications to nonequilibrium steady state
Abstract: For high dimensional case with multiple attractors, both chemical master equation and singular-perturbed diffusion processes would arise a local-global landscape confliction in the limit of zero noise, and a Markov jumping process emerges. Its nonequilibrium steady state corresponds to a discontinuity in the local landscape.

A9: Speaker: D. Limmer, University of California, Berkeley
Coauthor: D. Chandler
Title: Effects of Confinement on the Freezing Transition of Water
Abstract: Using a combination of molecular dynamics and field theoretic techniques, we have studied the freezing transition of water confined to nanometer sized hydrophilic pores. We find in agreement with experimental measurements and thermodynamic predictions that the melting temperature scales inversely with pore size for large pores. This scaling is recovered theoretically within a mean field limit of an interacting field theory. For small pores, the melting temperature exhibits a stronger pore size dependence and no freezing transition is observed for pores smaller than a critical pore size. This behavior is captured quantitatively with the introduction of fluctuations into the field theory. Further, the structure of the interface has been characterized within the field theory and molecular dynamics simulations.

A10: Speaker: U. Pedersen, University of California, Berkeley
Coauthor: D. Chandler
Title: Statistics of density fluctuations in supercooled viscous liquids
Abstract: Small length scale density fluctuations in normal homogeneous liquids obey gaussian statistics over many orders of magnitude. This dependence underlies successful theories of normal liquids. Here, we examine the statistics of density fluctuations outside the realm of normal liquids, in particular for atomistic models of structural glass formers - both non-associated and networked. We use enhanced sampling methods to compute probability distributions of density fields, and we consider a range of length scales and amplitudes. We find that gaussian statistics persists to a remarkable extent, even in the supercooled regime.

A11: Speaker: M. Mungan, Bogazici University
Coauthor(s): C. Yolcu
Title: Frenkel-Kontorova Models, Pinned Particle Configurations and Burgers Shocks
Abstract: Using an exactly solvable model, I will describe the relationship between the lowest energy configurations of an infinite harmonic chain of particles in a periodic potential and the evolution of characteristics in a periodically-forced inviscid Burgers equation. Physically, the shock discontinuities in the Burgers evolution arise from thermodynamical considerations and play an important role as they separate out flows related to lowest energy configurations from those associated with higher energies.
References:
1. M. Mungan and C. Yolcu, Phys. Rev. B 81 224116 (2010).
2. H.R. Jausslin, M.V.Kreiss and J.Moser, Proc. Symp. Pure Math. 65, 133 (1999)
3. W.E, Comm. Pure Appl. Math, 52, 811 (1999).
4. W.E, K.Khanin, A.Mazel and Ya.Sinai, Ann. Math. 151, 877 (2000).

A12: Speaker: M. Ha, Chosun University
Coauthor: H. Park
Title: Contact Process with Long-term Memory and Branching Bias

Abstract: We revisit a directed percolation (DP)-based yclically coupled model with branching bias, namely the driven contact process with power-law decay feedback (DCPP), where we can directly control not only the memory strength but also its power-law tail exponent as well as the preferred direction of branching. The CPP (without branching bias) in a one-dimensional lattice exhibits continuous varying scaling behaviors, which seems to result from long-term memories (power-law type feedbacks). In order to discuss the universality class of the CPP, we check whether an external driving is relevant to such critical scaling behaviors or not. Introducing branching bias in the CPP, we show that it changes both the continuously varying scaling regime and the critical decay exponent value. Based on our extensive simulation data and fine numerical analysis techniques, we argue that the DCPP belongs to the different universality class of the CPP, which implies that the universality class of the CPP is not DP. In addition, we find that the role of long-term memories in the CPP is somewhat similar to single particles in the pair contact process with diffusion (PCPD). As a result, we apply the conclusion of the CPP study to the discussion about the universality class of the PCPD. Finally, we discuss the mean-field behavior of the CPP, which is numerically tested and confirmed in quenched and annealed random networks.

A13: Speaker: M. Beceanu, Rutgers University
Title: Dispersion in Schrödinger's equation
Abstract: I am going to present several recent results concerning quantitative measures of dispersion in Schroedinger's equation: pointwise decay, wave operator boundedness, and Strichartz estimates. Some of these estimates are obtained jointly with Michael Goldberg, some are obtained jointly with Avy Soffer, and some are just the result of my own work.

A14: Speaker: M. Kiessling, Rutgers University
Title: Typical gravitating states on the 2 sphere
Abstract: N body systems interacting with Newtonian gravity on the 2 sphere exhibit interesting gravithermodynamic behavior in the limit as N goes to infinity. The microcanonical ensemble can be evaluated exactly with elementary functions, showing a second order phase transition. The microcanonical subensemble at fixed angular momentum does not yield an exactly solvable PDE, but it can be proved that it exhibits a phase transition, too, presumably of second order as well.

A15: Speaker: A. Vershynina, University of California, Davis
Coauthor(s): B. Nachtergaele and V. Zagrebnov
Title: Lieb-Robinson bounds and existence of thermodynamic limit for a class of irreversible quantum dynamics
Abstract: We consider a class of irreversible dynamics for quantum lattice systems with time dependent generators that are sums of Hamiltonian and dissipative terms that satisfy a suitable decay condition in space. For such models we prove Lieb-Robinson bounds and show the existence of the thermodynamic limit of the dynamics in the sense of a strongly continuous cocycle of unit preserving completely positive maps.

A16: Speaker: K. Korolev, MIM
Coauthor: D.R. Nelson
Title: Competition and cooperation in one-dimensional stepping stone models
Abstract: Cooperative mutualism is a major force driving evolution and sustaining ecosystems. Although the importance of spatial degrees of freedom and number fluctuations is well-known, their effects on mutualism are not fully understood. With range expansions of microbes in mind, we show that, even when mutualism confers a distinct selective advantage, it persists only in populations with high density and frequent migrations. When these parameters are reduced, mutualism is generically lost via a directed percolation process, with a phase diagram strongly influenced by an exceptional DP2 transition. The loss of mutualism is driven by spatial demixing of genotypes due to number fluctuations and short range migrations.

A17: Speaker; J. Frank, MIT
Coauthor: M. Kardar and J. Guven
Title: Turing patterns on curved surfaces
Abstract: We consider reaction-diffusion systems on curved surfaces. By applying Rayleigh-Schroedinger operator perturbation theory to the Laplacian on a Riemannian manifold, we find corrections to the eigenvalues and eigenfunctions of the Laplacian. The curvature-induced modifications to diffusion change the resulting Turing patterns, and can cause the patterns to lock onto geometric features of the surface. On a rippled cylinder, when the most unstable wavelength is nearly commensurate with the ripples, the Turing pattern aligns with peaks or troughs in a predictable manner.

A18: Speaker: O. Kogan, University of Pennsylvania
Coauthors: M. Dykman
Title: Rare fluctuations in nonequilibrium systems: onset of singularities in the path distribution
Abstract: Fluctuations in systems away from thermal equilibrium have features that have no analog in equilibrium systems. One of such features concerns large rare excursions far from the stable state in the space of dynamical variables. For equilibrium systems, the most probable fluctuational trajectory to a given state is related to the fluctuation-free trajectory back to the stable state by time reversal. This is no longer true for nonequilibrium systems, where the pattern of the most probable trajectories generally displays singularities. Here we study how the singularities emerge as the system is driven away from equilibrium, and whether there is a threshold for their onset. Using a resonantly modulated nonlinear oscillator as a model, we show that the singularities can emerge without a threshold if it takes an infi-

nite time for the system to go to infinity along the optimal path in thermal equilibrium. We find the scaling of the location of the singularities as a function of the control parameter. If the system reaches infinity in finite time, there is a threshold for the onset of singularities, which we study for the model.

Session B

B1: Speaker: S. Ji, Rutgers University
Title: Isomorphism between atomic physics and cell biology: Experimental evidence
Abstract: Isomorphism between atomic physics and cell biology: Experimental evidence. Sungchul Ji, Department of Pharmacology and Toxicology, Ernest Mario School of Pharmacy, Rutgers University, Piscataway, N.J. 08855 The statement that the living cell is the atom of biology is generally regarded as a mere metaphor, but, in this talk, I present the experimental evidence that the atom-cell relation is supported by a mathematical equation derived from the Planck radiation law which successfully explained the blackbody radiation data in 1900. See http://www.math.rutgers.edu/events/smm/smm105ji-abs.pdf for full abstract

B2: Speaker: K. Majumdar, Rutgers University
Coauthors: S. Ji, J. Rhyu, K. Bauiloor, D. Patel and R. Shah
Title: Interaction between Quantum States of Enzymes and Cell States in Budding Yeast during Glucose-Galactose Shift
Abstract: The single-molecule enzymological data on cholesterol oxidase (CO) measured by Xie and Lu [1] were found to fit the blackbody radiation-like equation (BRE) of the form, y = (a/(Ax + B)x5)/((e^(b/(Ax + B)) – 1), where a, b, A and B are constants and the meaning of x and y varies depending on the specific experiments under consideration [2]. Just as the fitting of blackbody spectral data into the Planck radiation formula entails quantizing the energy level of electrons in atoms, so the fitting of the enzymic activity data of CO to BRE indicates that the Gibbs free energy level of CO is quantized [3]. It was surprising to find that the protein stability data [3] and DNA microarray data measured from budding yeast undergoing glucose-galactose shift also fit BRE [4]. These observations taken together indicate to us that thermal fluctuations play a fundamental role in accessing the quantum states available to proteins, enzymes, and living cells. The quantum states of biopolymers and cells and the role of thermal fluctuations in accessing them can be combined into a coherent mechanistic scheme referred to as the ‘triadic signal transducing unit’ (TSTU) or ‘triadic information processing unit’ (TIPU) [3] that consists of three general steps: See http://www.math.rutgers.edu/events/smm/smm105majumdar.pdf for full abstract.

B3: Speaker: W. Szafran, Rutgers University
Coauthor(s): S. Ji, J. Rhyu and K. So
Title: Topology of Gibbs free energy landscape of living cells inferred from kinetics of genome-wide RNA metabolism
Abstract: The hypothesis that the Gibbs free energy levels of biopolymers are quantized is supported by two recent observations: (i) The single-molecule enzymological data of cholesterol oxidase [1] fit an equation similar in form to the blackbody radiation formula of M. Planck [2, 3] (see S. Ji, K. Majmudar, et al., Short Talks, this Conference), and (ii) the protein stability data [4] also fit the blackbody radiation-like equation (BRE) [3]. See http://www.math.rutgers.edu/events/smm/smm105szafran.pdf for full abstract.

B4: Speaker: J. Luo, Boston University
Coauthor(s): L. Xu, S. Buldyrev, C. Austen Angell, H.E. Stanley
Title: Liquid-Liquid Phase Transition in Modified Jagla Potential
Abstract: Jagla model of liquids which consists of particles interacting via a spherically symmetric two-scale potential with both repulsive and attractive ramps, is widely studied in simulations of liquids.
In recent study by Xu. et al, the Jagla model of liquids displays
anomalies similar to liquid water, and has the Liquid-Liquid phase transition and dynamics crossover, and leads to the location of the second critical point, which in their case, is above the melting line. However, in their study, the coexistence line of the Jagla model shows a positive slope, which is the opposite to what has been found in the experiments of water.
Recent work by Wilding. et al, uses Morte Carlo simulations to
study the modified Jagla model with different parameters. Their study indicates the possibility of changing slope of the coexistence line by modifying the Jagla potential.
We use the Discrete Molecular Dynamics (DMD) to study the Liquid-Liquid phase transition and dynamics of the modified
Jagla potential models.We find that the coexistence line can have negative slope in certain models, similar to water, and also the Widom line, based on both the compressibility K_T and specific heat C_P maximum locus, also shows negative slope. We further find out that the KT maximum line passes through the nose of the Temperature Maximum Density (TMD) line, while the CP maximum line ends in the glass transition region. Besides, these models show density anomalies of water and dynamics crossover. In summary, we succeed in obtaining a simple spherically symmetric two-scale potential model to represent the liquid water phase transition phenomena and anomalies, which hugely implements the previous Jagla model to make it more water-like.

B5: Speaker: V. Tkachenko, Ben-Gurion University of the Nagev, Israel
Title: On gaps in spectra of 1d periodic selfadjoint differential operators
Abstract: See http://www.math.rutgers.edu/events/smm/tkachenko-abs.pdf for abstract.

B6: Speaker: A. Laryea, CII
Title: Capital adequacy in financial services

Abstract: Explain how capital adequacy will affect the financial services in their operations and in the ration industry to attract multinational businesses.

B7: Speaker: T. Luchko, Rutgers University
Title: Ionic Atmosphere of DNA Calculated by Molecular Theory of Solvation
Coauthors: I. S. Joung, D. A. Case
Abstract: We present initial results on the structure of ionic atmosphere around DNA using the 3D-reference interaction site model (RISM) theory of molecular solvation. The method calculates the equilibrium 3D distribution of the solvent and is able to reproduce excess ion condensation observed in experiment.

B7[A] Speaker: D. Corradini, Boston University
Coauthors; S. V. Buldyrev, P. Gallo and H. E. Stanley
Title: Effect of hydrophobic solutes on the liquid-liquid critical point
Abstract: Jagla ramp particles, interacting through a ramp potential with two characteristic length scales, are known to show in their bulk phase thermodynamic and dynamic anomalies, similar to what is found in water. Jagla particles also exhibit a line of phase transitions separating a low density liquid phase and a high density liquid phase, terminating in a liquid-liquid critical point in a region of the phase diagram that can be studied by simulations. Employing molecular dynamics computer simulations, we study the thermodynamics and the dynamics of solutions of hard spheres (HS) in a solvent formed by Jagla ramp particles. We consider the cases o HS mole fraction $x = 0.10$, 0.15, and 0.20, and also the case $x = 0.50$, a 1:1 mixtureof HS and Jagla particles . We find a liquid-liquid critical point, up to the highest HS mole fraction; its position shifts to higher pressures and lower temperatures upon increasing x. We also find that the diffusion coefficient anomalies appear to be preserved for all the mole fractions studied.

B7[B]: Speaker: Y. Tu, Boston University
Coauthors: H.E. Stanley
Title: Liquid-liquid phase transition from a coarse-grained water model
Abstract: Positive and negative slopes of Widom lines are present in a coarse-grained water model. Here, the formation of H-bonds is coarse-grained by some with nearly tetrahedral orientation of H-bonding (the zeroth-order approximation) and some deviating far from the tetrahedral (the first-order approximation). This simple model reproduces the liquid-liquid phase transition, from whose critical point emanates the Widom line with negative slope along the maxima of heat capacity (CP). Surprisingly, when this model ignores the first-order approximation and returns back to the model only with the zeroth-order approximation, the Widom line holds its positive slope along the CP maxima, but its thermal anomalies go out from a range enclosed with density maxima and minima, gradually fades away and the critical point disappears.

B8: Speaker: J. Chen, Cornell University
Title: Statistical mechanics of Bose gas in Sierpinski carpets
Abstract: We investigate the equilibrium thermodynamics of massless and massive bosons confined in generalized Sierpinski carpets (GSCs), a class of infinitely ramified fractals having non-integer dimensions. Based on the uniqueness of Brownian motion on GSCs, as well as the state-of-the-art estimate of the heat kernel, we can, for the first time, make concrete calculation of the spectral zeta function, which is then used to construct the bosonic partition functions. For physical applications, we will describe blackbody radiation and Casimir effect in the fractal boxes, and state the criterion for Bose-Einstein condensation in terms of the transience property of the Hamiltonian operator.

B9: Speaker: Y. Baek, KAIST
Coauthor(s): M. Ha and H. Jeong
Title: Absorbing states of zero-temperature Glauber dynamics in quenched random networks
Abstract: We study zero-temperature Glauber dynamics in quenched Erdős-Renyi networks with random zero-magnetization initial states. It is found that its relaxation process exhibits large sample-to-sample fluctuations. In particular, the steady-state active link density is broadly distributed, as there are multiple absorbing states reachable by the system. In order to determine the likelihood of those absorbing states, we examine the probability distribution profile of the active link density at saturation as both the system size N and the average degree vary. Our results suggest that 'in the thermodynamic limit when the system size N goes to infinity as keeping the fixed value of the average degree , the system reaches an absorbing state with macroscopically large active link density, which is solely determined by .

B10: Speaker: C. Schreck, Oregon State University
Coauthors: T. Bertrand, M. Shattuck, C. O'Hern
Title: Vibrational density of states for granular solids
Abstract: It was recently shown that granular packings composed of frictionless particles with purely repulsive contact interactions are strongly anharmonic. When perturbed along an eigenmode of the static packing (in the harmonic approximation), energy leaks from the original mode of vibration to a continuum of frequencies even when the system is under significant compression due to the breaking of the weakest contact. In light of this, we perform numerical simulations to measure the displacement matrix averaged over fluctuations and the associated eigenspectrum of weakly vibrated frictionless packings, which possess well-defined equilibrium positions that are different than those of the nearest static packing. We find that there is an increase in the number of low-frequency eigenmodes of the displacement matrix in the harmonic approximation (over the number of low-frequency modes in the static case) and these modes provide

a more accurate description of the system dynamics. We also investigate the extent to which these results hold for systems with continuous potentials with repulsive and attractive interactions.

B11: Speaker: A. Ballard, University of Maryland
Coauthor(s): C. Jarzynski
Title: Replica exchange sampling with nonequilibrium switches Abstract: Efficient equilibrium simulation of complex systems is often hindered by large free energy barriers, preventing transitions between stable regions of phase space. Replica exchange (parallel tempering) has emerged as a powerful algorithm to overcome these difficulties. We introduce a replica exchange method in which attempted configuration swaps are generated using nonequilibrium work simulations. By effectively increasing phase space overlap, this approach mitigates the need for many replicas. We illustrate our method by using a model system and show that it is able to achieve the computational efficiency of ordinary replica exchange, using fewer replicas.

B12: Speaker: B. Young, Rutgers University
Title: On the N Body Foundations for the Relativistic Vlasov-Poisson Equations
Abstract: We consider the dynamics of an overall neutral two-specie Coulomb plasma with 2N charges as N goes to infinity. On the usual Vlasov time scale the familiar relativistic Coulombic Vlasov-Poisson two-specie system is obtained if the particles of each specie are initially chosen IID with specie-dependent distributions. If all particles are chosen IID by the same distribution this Vlasov dynamics reduces to trivial free-streaming of all particles, with identical particle distributions for all later times (on this Vlasov scale). To see non-trivial plasma dynamics in the latter case, we introduce the appropriate time and space scaling and find evidence for both, a dissipative operator and a gravitational-type Vlasov force term which govern the dynamics of an effective one-specie system. Interestingly, this dynamics suggests a compromise between the traditionally expected collisional kinetic evolution of “relativistic Lenard-Balescu-type" and the relativistic Newtonian Vlasov-Poisson evolution conjectured by Kiessling and Tahvildar-Zadeh for these plasmas.

B13: Speaker: P. Patrone, University of Maryland
Coauhor(s): D. Margetis, R. Wang
Title: Small fluctuations in epitaxial growth via conservative noise
Abstract: We study the joint effect of growth (material deposition from above) and nearest-neighbor entropic and force-dipole interactions in a stochastically perturbed system of N line defects (steps) on a vicinal crystal surface in 1+1 dimensions. We formulate a general model of conservative white noise, and we derive formulas for the terrace width distribution (TWD) and pair correlations, particularly the covariance matrix of terrace widths, in the limit $N \rightarrow \infty$; for small step fluctuations. We apply our formalism to two specific noise models which stem from respectively: (i) the fluctuation-dissipation theorem for diffusion of adsorbed atoms, and (ii) the phenomenological consideration of deposition-flux-induced asymmetric attachment and detachment of atoms at step edges. We discuss implications of our analysis, particularly the connection of noise structure to terrace width correlations, the behavior of these correlations in the macroscopic limit, and the comparison of our perturbation results to a known mean field approach (Phys. Rev. E 82 061601).

B14: Speaker: M. Krüger, MIT
Coauthor(s): T. Emig, G. Bimonte and M. Kardar
Title: Non-equilibrium Casimir force for two spheres
Abstract: The original Casimir effect, leading to attractive forces between objects at close proximity, considers quantum-zero-point fluctuations. At finite temperatures, additionally thermal fluctuations contribute to the force. In this talk, we discuss the non-equilibrium situation, where the objects as well as the enclosing environment have different temperatures. For the case of two spheres we demonstrate a collection of interesting effects which are absent in equilibrium.

B15: Speaker: A. Singha Roy, Indiana University
Title: Multiscale Simulations of Classical Nanosystems

Session C

C1: Speaker: J. Armas-Perez, UNAM
Coauthor(s): J. Quintana
Title: Numerical evidence for nematic and smectic behavior of two-dimensional hard models
Abstract: Mesophases of two infinitely hard models with chiral and anisotropic characteristics in two dimensions were studied. Nematic and smectic phase behavior were provided using Monte Carlo simulations for different values of the molecular parameters. Both models are geometrically chiral but one has polar structure. The isotropic-nematic phase transition (I-N) satisfies the features of the Kosterlitz Thouless type and the transition density was calculated using the Frank constant. Parallel and perpendicular distribution functions were computed to determine nematic-smectic phase transition (N-Sm). The nematic and smectic phases show signs of quasi long range order (QLRO).

C2: Speaker: J. A. Martinez Gonzalez, UNAM
Coauthor(s): J. Quintana, S. Varga and P. Gurin
Title: Nematic and smectic order in two-dimensional systems of v-shape molecules

Abstract: The nematic and smectic order in two dimensional systems of hard bent particles has been studied by means of the Onsager theory and Monte Carlo simulations. We found that the occurrence of both phases depends on the bent angle of the particle: in the hard needle limit we found the nematic phase, while increasing the bent angle the effects due to the excluded area lead to the smectic phase. The results obtained by both methodologies are in good agreement.

C3: Speaker: D. Gonzalez, University of Maryland
Coauthor: A. Pimpinelli and T. L. Einstein
Title: Maximum entropy method for the point-Island model in epitaxial growth
Abstract: We show that the maximum entropy method (MEM) can be used to describe some structural properties of the point-island model for epitaxial growth. In particular, we use the MEM to find an excellent analytical approximation for the gap size distribution, p(s) in 1D and for the capture zone distribution P(s) in 2D. We confirm that the equations derived with the MEM agree well with numerical results from simulations of the point island model [1].
[1] D. L. Gonzalez, A. Pimpinelli and T. L. Einstein, Submitted to PRE. This work was supported by the NSF-MRSEC at the University of Maryland, Grant No. DMR 05-20471 and a DOE CMCSN grant, with ancillary support from CNAM.

C4: Speaker: E. Vatansever, Dokuz Eylul University
Coauthor: G. Gulpinar
Title: Dynamic susceptibility of the metamagnetic Ising model near the critical point
Abstract: The magnetic relaxation of a metamagnetic Ising model is calculated within the framework of statistical equilibrium theory and the thermodynamics of irreversible processes. By making use of the mean-field expression for the magnetic Gibbs energy, the magnetic Gibbs energy production due to the irreversible process is calculated and time derivatives of the total and staggered magnetizations are treated as fluxes conjugate to their appropriate generalized forces in the sense of linear response theory. The kinetic equations are obtained by introducing kinetic coefficients that satisfy the Onsager reciprocity relation. By solving these equations an expression is derived for the dynamic or complex staggered susceptibility. Finally, magnetic dispersion and absorption factor are calculated and analyzed from the real and imaginary parts of AC staggered susceptibility in the neighbourhood of the critical point.

C5: Speaker: C. Aron, Rutgers University
Coauthor(s): G. Biroli and L. Cugliandolo
Title: Symmetries and broken symmetries of Langevin processes: fluctuation theorems
Abstract: The dynamics of classical system in interaction with a thermal bath can often be described by Langevin processes. We deal with multiplicative and colored noise. We present a study of the symmetries of the generating functionals (Martin-Siggia-Rose-Janssen-deDominicis) associated to these processes, in and out of equilibrium. At the level of observables, a first symmetry imply equations a la Schwinger-Dyson. A second one, valid only in equilibrium, gives all the equilibrium theorems. Broken out-of-equilibrium, it naturally gives rise to all the fluctuation theorems.

C6: Speaker: J. Barton, Rutgers University
Title: Phase diagram of generalized ABC model on interval
Abstract: We study the equilibrium phase diagram of a generalized ABC model on the interval of the one-dimensional lattice. This is a model of three particle species which interact via a mean field non-reflection-symmetric pair interaction, which need not be invariant under cyclic permutation of the particle species as in the standard ABC model studied earlier. We prove in some cases and conjecture in others that the scaled infinite system has a unique density profile except for some special values of the particle densities when the system undergoes a second order phase transition at a certain critical temperature.