



THE RAYMOND AND BEVERLY
SACKLER CENTER
FOR COMPUTATIONAL MOLECULAR
AND MATERIALS SCIENCE

Classical and Quantum Non- Equilibrium Dynamics

August 07, 2016 - August 10, 2016

Tel Aviv University, The Porter School Building (Auditorium), Tel Aviv, Israel

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Presentation Abstracts

Normal and Anomalous Diffusion of Atoms in Real Space and Frequency Space

Nir Davidson, Weizmann Institute of Science, Israel

I will describe three experimental systems where normal and anomalous diffusion of atoms are manifested by fat-tail distributions. The first involves ultra-cold atoms propagating in a 1D dissipative optical lattice showing anomalous dynamics both in real space and in momentum space. We show fractional self-similarity, fat-tail spatial distribution, persistence of phase-space correlations and power-law decay to equilibrium. The second system involves electro-magnetic induced transparency (EIT) of hot atoms diffusing in a hot vapor cell. We show that for one and two spatial dimensions the probability of a diffusing particle to return to origin is zero ("polya theorem") yielding time-correlation functions with diverging moments, leading in turn to fat-tail EIT spectra. The third system involves microwave "atomic clock" spectroscopy of ultra-cold dense atomic ensembles where s-wave atomic collisions yield normal and anomalous diffusion in frequency space leading to either increase or decrease of the atomic coherence times.

Irreversibility and Non-equilibrium Fluctuations at the Nanoscale: Dynamic Relaxation of a Levitated Glass Bead

Christoph Dellago, University of Vienna, Austria

Fluctuation theorems and non-equilibrium work relations, exact results obtained recently that characterize the fluctuations of heat, work and entropy in non-equilibrium processes, have significantly improved our understanding of how the Second Law of Thermodynamics operates at the nanoscale. Here, we apply this framework to investigate the fluctuations in relative entropy production for the relaxation of a laser-trapped nanoparticle from a non-equilibrium steady state towards equilibrium. Because of the low damping, the dynamics of this nanomechanical system can be precisely controlled and the oscillator can be cooled by parametric feedback. Based on the steady state distribution, which is determined analytically based on the equations of motion of the system, we determine the change of relative entropy observed after the feedback has been switched off. The statistics of heat transfer measured in repeated relaxation experiments obeys a fluctuation theorem derived for this particular situation. We discuss the relevance of our work for the study of transitions between arbitrary non-equilibrium steady states.

The Micromechanics of Cellularized Biopolymer Materials

Herbert Levine, Rice University, Texas, USA

Tissues are composed of cells embedded in a fibrous matrix made up of a variety of proteins such as collagen. These materials exhibit highly nonlinear elastic behavior as well as irreversible dynamical changes when acted upon by the active contractile machinery of the cells. This talk will introduce a simple lattice-based model of these materials and compare micro-rheology predictions with data taken using optical tweezer techniques for a gel composed of cancer cells embedded in a collagen matrix.

Finding a New Job for Maxwell's Demon: Improving Free Energy Calculations

Saar Rahav and Shahaf Asban, Technion - Israel Institute of Technology, Israel

Our understanding of small out-of-equilibrium systems have undergone a revolution in the last two decades, with the development of stochastic thermodynamics. It was found that small systems driven away from equilibrium satisfy the Jarzynski equality. This equality can be used to determine free energy differences from repetitions of a non-equilibrium process. However, such calculations are known to suffer from poor convergence. The deep connections between information and thermodynamics have also been extensively studied. Information engines, where measurement and feedback allow to extract additional work from a system, have been studied theoretically and realized in experiments. It is only natural to wonder whether measurement and feedback can also be useful in free energy estimation. We argue that measurement and feedback can greatly improve the convergence of such calculations, and furthermore show how the information gained from the measurement can be used for that purpose. We study numerically a pulling process of a DNA hairpin, modeled as a two-state system, as a test case for our approach.

Dynamics and Statics of Three-Dimensional Jamming Percolation

Yair Shokef, Tel Aviv University, Israel

By analyzing initial configurations in kinetically-constrained lattice models we theoretically predict their resultant dynamics. We employ an iterative culling procedure in order to find the number of particles blocking each particle, and then relate that to the persistence time, namely the time of first motion (lattice gas) or spin flip (Ising model). Our theoretical analysis perfectly agrees with numerical simulations of the Fredrickson-Andersen and Kob-Andersen models in one and two dimensions, as well as with the two-dimensional spiral model. The second aspect of our dynamical predictions focuses on our extension of the spiral model to three dimensions, for which we identify that jamming and caging are two decoupled physical phenomena. At a first critical density a finite fraction of the particles in the system are permanently jammed and do not move, while only at a higher critical density, do the mobile particles become caged and self-diffusivity vanishes.

Universal Statistics of Low-frequency Vibrational Modes in Disordered Solids

Eran Bouchbinder, Weizmann Institute of Science, Israel

Low-frequency vibrational modes play a central role in determining various fundamental properties of glasses, yet their statistical and mechanical properties are far from understood. Using extensive numerical simulations of several model glasses in three dimensions, we show that in systems of linear size L sufficiently smaller than a crossover size L_D , the low-frequency tail of the density of states follows $D(\omega) \sim \omega^4$ up to the vicinity of the lowest Goldstone mode frequency. We find that the sample-to-sample statistics of the minimal vibrational frequency in systems of size $L < L_D$ is Weibullian, with scaling exponents in excellent agreement with the universal ω^4 law. We further show that the lowest frequency modes are spatially quasi-localized, and that their localization and associated quartic anharmonicity are largely frequency-independent. The effect of non-equilibrium preparation protocols on the low-frequency modes is elucidated and a number of glassy lengthscales are defined. Future directions are briefly discussed. Work with Edan Lerner (Amsterdam) and Gustavo During (Santiago)

Force Chains and Force Laws in Granular Systems

Itamar Procaccia, Weizmann Institute of Science, Israel

In this talk I will consider three related problems. First, **the determination of the normal and transverse (frictional) inter-particle forces** within a granular medium is a long standing, daunting, and yet unresolved problem. I will present a new formalism which employs the knowledge of the external forces and the orientations of contacts between particles (of any given sizes), to compute all the inter-particle forces.

Having solved this problem we exemplify the efficacy of the formalism showing that the force chains in such systems are determined by an expansion in the eigenfunctions of a newly defined operator. Second, **the problem of how to determine the force laws** in an amorphous system of interacting particles. Given the positions of the centers of mass of the constituent particles I will show a new algorithm to determine the inter-particle force-laws. Having n different types of constituents we determine the coefficients in the Laurent polynomials for the $(n+1)/2$ possibly different force-laws. A visual providing the particle positions in addition to a measurement of the pressure is all that is required. The algorithm proposed includes a part that can correct for experimental errors in the positions of the particles. Such a correction of unavoidable measurement errors is expected to benefit many experiments in the field. Third and last, in glassy thermal systems I will show how to **find the effective forces that keep the average positions** of the particles. These effective forces depend on the temperature and open up new vistas for the understanding of thermal amorphous systems.

Response-Correlation Inequality in Dynamical Systems

Eytan Katzav, the Hebrew University of Jerusalem, Israel

The flurry of activity in non-equilibrium statistical phenomena covers many fields of theoretical and practical importance such as critical dynamics, growth models, front propagation, crack propagation and many more. We will discuss an exact inequality relating the response function, measuring the steady state response of the physical field of interest to an external probe, and the correlation function. This inequality generalizes the Schwartz-Soffer inequality derived for quenched random systems. When turned then into an exponent inequality, an interesting classification into two classes of dynamical systems is obtained - where different yet complementary exponent inequalities are found. These inequalities bear important consequences for a wide set of dynamical problems, including critical dynamics and KPZ-like problems.

Nonequilibrium Charge Transport in Molecular Junctions: Vibrational Effects and Transient Phenomena

Michael Thoss, University of Erlangen-Nuremberg , Germany

Molecular junctions, i.e. single molecules bound to electrodes, are interesting systems to study nonequilibrium quantum transport at the nanoscale. An important transport mechanism in molecular junctions is electronic-vibrational coupling. In this talk, various aspects of vibrationally coupled electron transport are analyzed, including current-induced vibrational excitation [1], nonadiabatic [2] and quantum interference [3] effects, as well as fluctuations [4]. Furthermore, transient phenomena and signatures of multistability in nonequilibrium transport are discussed [5]. The studies employ a combination of generic as well as first-principles based models and different transport methods, including nonequilibrium Green's functions and the multilayer multiconfiguration time-dependent Hartree method [6]. The latter method, which allows a numerically exact treatment of the time-dependent transport problem, can be combined with density matrix approaches [5] and provides benchmark results for approximate approaches.

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[4] C. Schinabeck, R. Härtle, H. B. Weber, M. Thoss, *Phys. Rev. B* 90, 075409 (2014).

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[6] H. Wang and M. Thoss, *J. Chem. Phys.* 131, 024114 (2009); 138, 134704 (2013).

Plasmon Controlled Molecular Junctions

Yoram Selzer, Tel Aviv University, Israel

The ability to squeeze light by means of plasmons into nano-scale metal gaps offers exciting possibilities to probe, control, switch, and gate the conductance of nano-scale and molecular junctions. I will present several experimental systems that demonstrate plasmonic steering of various conductance processes within molecular and single atom junctions. Initial results demonstrating experimental capabilities to perform ultrafast (~70 fsec resolution) time resolved conductance measurements of molecular junctions will also be shown.

Taming the Dynamical Sign Problem in Quantum Many-body Systems: Advances in Inchworm Monte Carlo

Guy Cohen, Tel Aviv University, Israel

Monte Carlo methods for calculating dynamics and out-of-equilibrium properties of quantum many-body systems suffer from a dynamical sign problem. This sign problem makes simulating real-time dynamics for long times exponentially hard. We recently proposed the "Inchworm Algorithm", which - by reusing information obtained in propagation to short times to extend the propagation to longer times - largely overcomes the dynamical sign problem, at least for a certain class of quantum many-body systems. The algorithm effectively changes the computational scaling in time from exponential to quadratic. We discuss the access it provides to quench dynamics and response to oscillating magnetic fields in the strongly correlated regimes of the Anderson impurity model; applications to several regimes of the spin-boson model; and ongoing work on applications to strongly correlated materials and molecules.

Dissipation Induced Topological Insulators: A Recipe

Moshe Goldstein, Tel Aviv University, Israel

It has recently been realized that driven-dissipative dynamics, which usually tends to destroy subtle quantum interference and correlation effects, could actually be used as a resource. By proper engineering of the reservoirs and their couplings, one may drive a system towards a desired quantum-correlated steady state, even in the absence of internal Hamiltonian dynamics. An intriguing class of quantum phases is characterized by topology, including the quantum Hall effect and topological insulators and superconductors. Which of these noninteracting topological states can be achieved as the result of purely dissipative Lindblad-type dynamics? Recent studies have only provided partial answers to this question. In this talk I will present a general recipe for the creation, classification, and detection of states of the integer quantum Hall and 2D topological insulator type as the outcomes of coupling a system to reservoirs, and show how the recipe can be realized with ultracold atoms and other quantum simulators. The mixed states so created can be made arbitrarily close to pure states, and the construction may be generalized to other topological phases.

Interplay Between Geometry and Dephasing and the Increase of Power Output in Photosynthetic Exciton Transfer Networks

Yonatan Dubi, Ben-Gurion University, Israel

The striking efficiency of energy transfer in natural photosynthetic systems and the evidence of long-lived quantum coherence in biological light harvesting complexes has triggered much excitement, due to the evocative possibility that these systems - essential to practically all life on earth - use quantum mechanical effects to achieve optimal functionality. A large body of theoretical work has addressed the role of local environments in determining the transport properties of excitons in photosynthetic networks and the survival of quantum coherence in a classical environment. Nonetheless, understanding the connection between quantum coherence, exciton network geometry and energy transfer efficiency remains a challenge. Here we address this connection from the perspective of heat transfer within the exciton network. Using a non-equilibrium open quantum system approach and focusing on the Fenna-Matthews-Olson complex (the "fruit-fly" of exciton transfer), we demonstrate that finite local dephasing can be beneficial to the overall power output. The mechanism for this enhancement of power output is identified as a gentle balance between quantum and classical contributions to the local heat flow, such that the total heat flow is directed along the shortest paths and dissipation is minimized. Strongly related to the spatial network structure of the exciton transfer complex, this mechanism elucidates how energy flows in photosynthetic excitonic complexes.

First Detection Time for a Quantum Walker

David Kessler, Bar-Ilan University, Israel

We investigate the statistics of the first detected passage time of a quantum walk. The postulates of quantum theory, in particular the collapse of the wave function upon measurement, reveal an intimate connection between the wave function of a process free of measurements, i.e. the solution of the Schrödinger equation, and the statistics of first detection events on a site. For stroboscopic measurements a quantum renewal equation yields basic properties of quantum walks. For example, for a tight binding model on a ring we discover critical sampling times, diverging quantities such as the mean time for first detection, and an optimal detection rate. For a quantum walk on an infinite line the probability of first detection decays like $(\text{time})^{-3}$ with a superimposed oscillation, critical behavior for a specific choice of sampling time, and vanishing amplitude when the sampling time approaches zero due to the quantum Zeno effect.

Classical and Quantum Non-equilibrium Dynamics of Nonlinear Nanomechanical Systems

Ron Lifshitz, Tel Aviv University, Israel

The study of the dynamics of driven and damped nonlinear mechanical resonators is regaining attention in recent years thanks to rapid developments in the fields of electro- and optomechanical systems in the micro and nano scales. Such resonators are typically characterized by very high frequencies, extremely small masses, and weak damping. As such, they are naturally being developed for a variety of novel applications such as sensing with unprecedented accuracy, but are also being used for studying fundamental physics at small scales—exploring mesoscopic phenomena, and even approaching full quantum behavior. Maybe less known is the fact that they are also being used for studying nonlinear dynamics under these conditions. The aim of this lecture is to provide an overview of some of the nonequilibrium dynamical phenomena observed in these systems, while highlighting the common concepts and theoretical tools that we have developed for dealing with them.

Intermediate Dynamic Length Scale in Complex Fluids

Haim Diamant, Tel Aviv University

Over sufficiently large distances any complex fluid responds as a continuous medium, characterized by bulk viscoelastic moduli. In other words, to us goo is just goo, not a collection of complicated structures inside water. But how large is "sufficiently large"? Close examination reveals a distinctive dynamic length scale, which in various complex fluids pushes the bulk behavior to distances much larger than the small-scale correlation length. In entangled F-actin networks this intermediate length was found to be of micron scale. We discuss its various manifestations in the dynamics of complex fluids and of objects embedded in them.

Statistical Physics of Stochastic Reaction Networks

Ofer Biham, the Hebrew University of Jerusalem, Israel

I will present recent results in the study of reaction networks. In the thermodynamic limit reaction networks can be described by rate equations based on the law of mass action. However, in the small-system limit the effect of fluctuations becomes important, calling for stochastic methods based on the master equation. I will characterize the different kinetic regimes and will show that moment equations provide an efficient method for the calculation of reaction rates in the stochastic limit. The application of this methodology to chemical networks in the interstellar space and to gene regulatory networks in cells will be discussed.

Statistics of Discrete Motor-driven Events in Reorganizing Active Networks

Yael Roichman, Tel Aviv University, Israel

Active materials inspired from biological systems are a paradigmatic model to study non equilibrium statistical mechanics. A common method to access their non-equilibrium statistics is to measure the fluctuation distribution of a tracer particle embedded in the material. Usually, discrete motor-induced events cannot be characterized in this way due to the multitude of active processes taking place simultaneously during measurement. Here we measure the statistics of such discrete events showing the appearance of distinct shoulders in the van Hove correlation function at high motor concentration. We do so by tailoring a model active system based on cytoskeleton proteins to maintain approximately steady-state dynamics over several hours. The shoulders' appearance coincides with a transition from steady-state dynamics to slowly evolving dynamics as the motor concentration increases. We further demonstrate how these discrete active events accumulate at longer lag times to a broadened Gaussian distribution.

Theory for Multi-motor Driven Nano-carriers with Application to Rational Design

Rony Granek, Ben-Gurion University, Israel

A rational design for a nano-particle is suggested, that will maximize the arrival efficiency from the plasma membrane to the nucleus surrounding. The design is based on grafting the particle surface with polymer spacers that end with motor protein associating molecules, e.g., nuclear localization signal peptides. It is theoretically shown that the spacer polymer molecular weight can be adjusted to significantly increase the effective particle processivity time. This should lead to appreciable enhancement of the active transport of the nano-carrier, and consequently drug delivery, to the nucleus [1]. Next we account for motor-motor coupling which may lead to stalling and jamming [2]. We first construct a simple, yet general, theoretical-phenomenological model for single motor (dynein or kinesin) motion. The model correctly predicts the motor step size distribution and its dependence on the load, as recently measured in single molecule experiments. Second, we began to use our proposed model to predict transport characteristics of multi-motor complexes: (i) First, we considered a chain of motors connected by springs, a recently studied construction for a pair. (ii) Second, we considered an array of motors all connected by identical springs to a stiff rod, which is closely related to standard gliding motility assays. In both systems, and for any number of carrying motors, we find that, while low flexibility results in a strongly damped velocity, increased flexibility renders an almost single motor velocity (in accord with experimental findings), thus allowing to achieve strongly enhanced cargo run lengths. The characteristic spring constant that controls this crossover behavior is the stalling force divided by the mean step size. Interestingly, in model (i) and in the large spring constant regime, we obtain a cooperative behavior. Recent results for the model spherical nano-carrier discussed above will be presented. On the cellular level, ample experimental evidence exists of the role of microtubules (MTs) in perinuclear localization of cellular components (e.g. Golgi cisternae), retroviruses, and adenoviruses. We explain this localization purely by dynein mediated active transport of cargos towards the centrosome, a process moderately mitigated by cytoplasmic diffusion [3]. We then generalize the model to include drug release from the NC, drug cytoplasmic diffusion, and nuclear uptake of the drug. We find that, so long as the characteristic drug dissociation time is of the order of, or longer than, the time to reach the steady state NC (perinuclear) distribution, the higher the processivity the faster is the drug accumulation in the nucleus. Further work will allow optimizing NC parameters for different target cells and drugs.

[1] O. Cohen and R. Granek, "Nucleus-Targeted Drug Delivery: Theoretical Optimization of Nanoparticles Decoration for Enhanced Intracellular Active Transport", *Nano Letters* 14, 2515-2521 (2014).

[2] I. Peker and R. Granek, *J. Phys. Chem. B, Articles ASAP*, DOI: 10.1021/acs.jpcc.6b02790.

[3] R. Orland and R. Granek, to be published.

Pressure in Active Systems

Yariv Kafri, Technion - Israel Institute of Technology, Israel

Pressure is the mechanical force per unit area that a confined system exerts on its container. In thermal equilibrium, the pressure depends only on bulk properties (density, temperature, etc.) through an equation of state. The talk will show that in non-equilibrium active systems containing self-propelled particles, the pressure instead can depend on the precise interactions between the system's contents and its confining walls. This implies that generic active systems have no equation of state. Implications of this result, as well as results for forces on general objects embedded in an active fluid, will be discussed.

Dynamics of Tracers within Living Cells and Active Gels

Nir Gov, Weizmann Institute of Science, Israel

Passive tracer particles that are embedded inside the cell cytoskeleton, and in artificial active gels, allow to probe the dynamics of these non-equilibrium systems. We developed the motion of a particle confined within a harmonic trap, and subject to random active forces. This model has been extended to describe a thermal trap that is moved actively around within a visco-elastic medium, and compares very well to observations of beads embedded in living cells. A model with a finite-depth trap can explain anomalous diffusion within an active gel, where the tracer can hop between trapping sites as the gel gets remodeled by the active forces. These models are compared to recent experiments.

Quantum and Classical Simulations of Enzymatic Reactions – Case Studies

Dan Major, Bar-Ilan University, Israel

Enzymes are fascinating biological macromolecules which catalyze chemical reactions at rates which approach the encounter rate between the enzyme and substrate. Studying the nature of enzyme catalysis is of great importance in order to appreciate Nature's achievement, develop synthetic catalysts, and design new inhibitors. Our current understanding of enzyme catalysis dates back to the early days of Linus Pauling who introduced the concept of a pre-organized active site, which provides preferential stabilization of the transition state. Although this concept remains the pillar of enzyme catalysis, there are numerous cases where other effects are at play. In the current talk, I will focus on several current challenges relating to statistical and non-statistical behavior in enzyme catalysis, which we have addressed using multi-scale simulation approaches in our group. In particular, I will discuss the role of non-statistical dynamics, conformational dynamics, and tunneling. These effects will be highlighted with three example systems: (1) Bornyl Diphosphate Synthase (BPPS) (2) Nitroalkane Oxidase (NAO), and (3) Dihydrofolate Reductase (DHFR). In BPPS the complex potential energy surface includes a bifurcation point, which results in a dynamically controlled reaction. For the NAO reaction, I show that there is a small catalyzing tunneling contribution. In the case of DHFR I present results indicating that standard transition state theory-like simulation methods produce incorrect transition states.

Chaos, Metastability and Ergodicity in Atomtronic Superfluid Circuits

Doron Cohen, Ben-Gurion University, Israel

We clarify the role of "chaos" for the metastability criteria of flow states [1], and for the possibility to witness Rabi oscillations in a SQUID-like setup [2]. We refer to coherent, as well as to stochastic-like features [3,4] in the dynamics and in the thermalization process.

[1] G. Arwas, A. Vardi, D. Cohen, *Scientific Reports* 5, 13433 (2015).

[2] G. Arwas, D. Cohen, *New Journal of Physics* 18, 015007 (2016).

[3] C. Khripkov, A. Vardi, D. Cohen, *New J. Phys.* 17, 023071 (2015).

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1. ***Information Machine***

Tamir Admon, Tel Aviv University, Israel

We propose a realization of an information machine which converts information to work, using the concept of Leo Szilard's feedback protocol. In our realization, a colloidal particle is drifting with fluid flow in a 1D channel until it encounters a barrier. The particle is monitored as it diffuses. Once it moves further enough upstream, the barrier is moved closer to the particle without affecting it. Repeating this feedback based action results in transporting the particle itself. We aim to implement this model both in experiment and in simulation. Our experimental design is comprised of a colloidal particle diffusing in a microfluidic channel, with a repelling laser based barrier. Here, we present preliminary results regarding the feasibility of such experiments. On the simulation front, we implement a Langevin dynamics simulation and study the relevant time scales of the system's dynamics. We also study the effect of sampling and feedback cycles on the efficiency of the information machine with measurement correlation consideration.

2. ***The Effect of Interactions and Disorder on the Relaxation of Two-level Systems in Amorphous Solids***

Ofek Asban, Ben-Gurion University, Israel

We study the slow relaxation of amorphous solids and how it is affected by disorder and interactions. At low temperatures the dynamical degrees of freedom in amorphous solids are tunneling two-level systems (TLS) which can be represented by the standard tunneling model (STM). We address an extension of the STM by adding the phonon mediated inter-TLS dipole interactions which we call the TLS-glass model (TG). We solve the linearized rate equations of the sites occupancies in the mean-field approximation. The total relaxation of the system is then obtained by the time dependence of the mean TLS occupations. The low energy density of states shows the expected pseudo-gap. We find $1/\lambda$ distribution of relaxation rates (where λ is the TLS-phonon relaxation rate), which become faster with enhanced disorder. All the above mentioned results are qualitatively similar to results found for the Electron-glass model (EG) within the same theoretical framework. However, the TG differs from the EG in that with enhanced interactions the dynamics become faster in the former and slower in the latter.

3. ***Local and Global Equilibrations in an Ubiquitous Integrable Ensemble (GGE)***

Robert Englman, Ariel University, Israel

Ensemble-time ergodicity is proven under some restrictive assumptions for a classical system, comprising interacting harmonic oscillators. An atom in a monatomic chain or lattice is shown to behave ergodically, in the sense that the time averaged behavior of a lattice point is identical to the ensemble average of the behavior of any lattice point at any long time (in large excess of the inverse vibrational frequencies). This equivalence (for "local observables") differs from the Fermi-Pasta-Ulam result for mode energies (which are nonlocal). In the quantum case the results are the same. Extensions exist to wider instances of interacting local systems, beyond the coupled harmonic lattice. The outcome can be seen in the contexts of Canonical Typicality and the Eigenstate Thermalization Hypothesis. Proposed experimental tests are through the second order Doppler shift in the Mossbauer effect and in the width of the optical absorption line shape in impurity spectra. The ensembles that are constructed in the theory are optimally "typical" for a minimal subsystem that is strongly coupled to a large surrounding. The integrable manifold of the coupled oscillators constitutes a Gibbs Generalized Ensemble. The exponential multipliers in this are derived and a Maximum Entropy distribution of the weights are obtained in a micro-canonical ensemble.

R. Englman, "Local ergodicity in coupled harmonic vibrators: classical and quantal treatments". J. Phys .A: Math. Theor. 49 (2016) 115102

4. ***Hierarchical Quantum Master Equation Approaches to Electronic-vibrational Coupling and Time-dependent Effects in Single-molecule Junctions***

André Erpenbeck, University of Erlangen-Nuremberg, Germany

The interaction between electronic and vibrational degrees of freedom as well as time-dependent effects are essential for understanding electron transport through single-molecule junctions. The hierarchical quantum master equation approach offers an, in principle, numerically exact solution to this transport problem. In this contribution, we demonstrate how the hierarchical quantum master equation approach can be used to describe time-dependent transport through a molecule influenced by the vibrational degrees of freedom. Thereby, we illustrate different possibilities to incorporate electronic-vibrational interactions in the HQME approach, ranging from the quasi-classical Ehrenfest approach to descriptions where the nuclear degrees of freedom are treated quantum mechanically. Employing representative model systems, the differences and limitations of the various approaches are highlighted. Furthermore, we investigate physical effects resulting from the time-dependencies or electronic-vibrational coupling in some detail.

5. ***Effect of Phonon Coupling on the Dynamics of Three Level System***

Dawit Hiluf Hailu and Yonatan Dubi, Ben-Gurion University, Israel

This work investigates the effect of phonon coupling on the transfer of population and creation of coherence using variant of stimulated Raman adiabatic passage (STIRAP) known as fractional stimulated Raman adiabatic passage (FSTIRAP). The study is based on the Liouville equation, which is solved numerically in the adiabatic limit. Although the phonon is assumed to be coupled only to the intermediate state, it is coupled to the other two states by dipolar system-environment interaction, inducing phonon coupling to the other states which are not directly in contact with the phonon. For the STIRAP pulse protocol, the efficiency of the transfer decreases exponentially with the electron-phonon coupling, until the coupling strength is strong enough to make the process fully incoherent, in which case the population transfer is 1/3 in each level. For the FSTIRAP protocol we find that the transferred population to target state decreases, leaving some population on the intermediate state. Consequently, there is an increase in the magnitude of the coherences ρ_{01} , ρ_{12} , albeit small.

6. ***Single Molecules Under Confinement - Breaking the Diffusion and Diffraction Limits***

Jonathan Jeffet, Tel Aviv University, Israel

Here we present two aspects of single molecules confinement to nanochannel array: The first, super resolution and accuracy enhancement of optical genome mapping in nanochannels by multi-frame analysis. Optical genome mapping in nanochannels is a powerful genetic analysis method complementary to DNA sequencing. The method is based on detecting a pattern of fluorescent molecules attached along individual DNA fragments, creating a fluorescent genetic barcode. Mapping resolution is limited not only by the optical diffraction limit but also by the thermal fluctuations of the DNA molecules suspended in the nanochannels. We utilize single-molecule super-resolution localization and tracking in order to directly define the mapping accuracy and resolving power of the technique. To facilitate these measurements we studied a naturally occurring genetic repeat array and labeled each repeat with Trolox conjugated fluorophores for extended photostability. We acquired long fluorescence time traces that experimentally validate the correspondence of confined DNA dynamics to the Odijk theory of confined polymer chains. Furthermore, we show how time-averaging and single-step photo-bleaching impact mapping accuracy enhancement and in some cases allow resolving sub-diffraction spaced fluorescent markers along the DNA. The second aspect is confinement of light driven nano-submarines to nanochannels for improved imaging and tracking capabilities. We utilize single molecule imaging of fluorescent submersible nano-machines, in order to assess whether sufficient amount of work could be exerted by the motor to propel the nano-machine and overcome the dominant viscosity forces in this extremely low Reynolds number regime. By tracking the nano-machines with and without motor activation in the channels, we characterize the difference in diffusion between activated and non-activated motor, and show a two fold increase in diffusion when the motor is activated.

7. ***Large Tunable Thermophase in Superconductor -- Quantum Dot -- Superconductor Josephson Junctions***

Yaakov Kleeorin, Ben-Gurion University, Israel

In spite of extended efforts, detecting thermoelectric effects in superconductors has proven to be a challenging task, due to the inherent superconducting particle-hole symmetry. Here we present a theoretical study of an experimentally attainable Superconductor -- Quantum Dot -- Superconductor (SC-QD-SC) Josephson Junction. Using Keldysh Green's functions we derive the exact thermo-phase and thermal response of the junction, and demonstrate that such a junction has highly tunable thermoelectric properties and a significant thermal response. The origin of these effects is the QD energy level placed between the SCs, which breaks particle-hole symmetry in a gradual manner, allowing, in the presence of a temperature gradient, for gate controlled appearance of a superconducting thermo-phase. This thermo-phase increases up to a maximal value of $\pi/2$ after which thermovoltage is expected to develop. Our calculations are performed in realistic parameter regimes, and we suggest an experimental setup which could be used to verify our predictions.

8. ***Faceting in Multi-walled Nanotubes***

Itai Leven, Tel Aviv University, Israel

Nanotubes hold great promise for the miniaturization of advanced technologies. Their exceptional physical properties are intimately related to their detailed morphological and crystal structure. Importantly, circumferential faceting of multiwalled nanotubes serves to reinforce their mechanical strength and alter their tribological and electronic properties. Here, nanotube faceting is fully rationalized in terms of interlayer registry patterns. We find that, regardless of the nanotube identity, faceting requires chiral angle matching between adjacent layers. Above a critical diameter that corresponds well with experimental findings, achiral multiwalled nanotubes display evenly spaced extended axial facets, the number of which is determined by the interlayer difference in circumferential unit cells. Elongated helical facets, most commonly observed in experiment, appear in nanotubes exhibiting a small interlayer chiral angle mismatch. In the case of uncorrelated wall chiralities faceting is suppressed and surface corrugation induced by the Moiré superlattice is obtained in excellent agreement with experiment. It is therefore evident that gaining control over their interlayer registry matching provides a route for the mechanical enforcement as well as tribological and electronic properties tuning of MWNTs.

9. ***Interlayer Potential for Graphene/h-BN Heterostructures***

Tal Maaravi, Tel Aviv University, Israel

The two dimensional heterostructure formed of graphene and hexagonal boron nitride (h-BN) exhibits rich physical properties and plays a central role in the field of nanotribology. In this study, a new interlayer force-field for layered graphene and h-BN based structures is presented. The force-field contains two terms representing the interlayer attraction due to dispersive interactions, and repulsion due to anisotropic overlaps of electron clouds. With appropriate parameterization against reference binding and sliding energy profiles obtained from density functional theory using a screened exchange hybrid functional augmented by a many-body dispersion treatment of long-range correlation, the potential is able to simultaneously capture well the binding and lateral sliding energies of planar h-BN and graphene based dimer systems. Furthermore, the transferability of the potential to multi-layered systems is demonstrated by considering the binding energy of bulk graphene/h-BN alternating stacks. The new developed force field thus enables the accurate and efficient modeling of the structural, mechanical, tribological, and dynamic properties of layered heterostructures based on graphene and h-BN.

10. ***Size Dependent Friction in Graphene/h-BN Heterojunctions***

Davide Mandelli, Tel Aviv University, Israel

Relevant for applications in nano- and micro-motive components is the search for robust incommensurate superlubric interfaces. At the moment heterojunctions of rigid layered materials seem [1,2] to be the best choice for such applications. Graphene (G) and hexagonal boron-nitride (h-BN) are promising candidates as they provide both adequate robustness and incommensurability, and are currently under investigation [3,4]. A detailed theoretical description of such system is therefore mandatory as it will serve as a solid background for the interpretation and

the design of future experiments. Here we present preliminary results of numerical simulations of the frictional properties of G/h-BN heterojunctions, performed adopting a recently developed inter-layer potential [5] for this heterostructure. In order to understand the relevant features determining the frictional response of the interface, we investigate the effects caused by variation of the interface relative angular misalignment, the external load and the size of hexagonally shaped graphene-flakes sliders. In the case of aligned flakes we observed an interesting non-monotonic behavior of friction versus size in the heterogeneous G/h-BN junction, which is explained by the appearance of the Moire pattern of the incommensurate interface. This also leads to the existence of a (load dependent) critical size at which the friction measured in G/G interfaces becomes larger than in G/h-BN. In rotated flakes friction reduces by 2-4 order of magnitudes, as expected, and for the sizes investigated no scaling is observed, in agreement with predictions of previous geometrical models. [6] More interestingly, misaligned G/h-BN interfaces are characterized by a smoother sliding than G/G interfaces, where friction is found to be significantly larger.

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11. ***Nanotubes Motion on Layered Materials: A Registry Perspective***
Inbal Oz, Tel Aviv University, Israel

At dry and clean material junctions of rigid materials the corrugation of the sliding energy landscape is dominated by variations of Pauli repulsions. These occur when electron clouds centered around atoms in adjacent layers overlap as they slide across each other. In such cases there exists a direct relation between interfacial surface (in)commensurability and superlubricity, a frictionless and wearless tribological state. The Registry Index is a purely geometrical parameter that quantifies the degree of interlayer commensurability, thus providing a simple and intuitive method for the prediction of sliding energy landscapes at rigid material interfaces. In the present study, we extend the applicability of the Registry Index to non-parallel surfaces, using a model system of nanotubes motion on flat hexagonal materials. Our method successfully reproduces sliding energy landscapes of carbon nanotubes on Graphene calculated using a Lennard-Jones type and the Kolmogorov-Crespi interlayer potentials. Furthermore, it captures the sliding energy corrugation of a boron nitride nanotube on hexagonal boron nitride calculated using the h-BN ILP. Finally, we use the Registry Index to predict the sliding energy landscapes of the heterogeneous junctions of a carbon nanotubes on hexagonal boron nitride and of boron nitride nanotubes on graphene that are shown to exhibit a significantly reduced corrugation. For such rigid interfaces this is expected to be manifested by superlubric motion.

12. ***Diffusion Under Time Dependent Stochastic Resetting***
Arnab Pal, Technion - Israel Institute of Technology, Israel

Stochastic Resetting is an intermittent search process which mixes local and long-range moves thus affecting the properties of a simple diffusion process. The questions raised can be of manifolds such as the statistical properties of this process, to be specific the characterization of the steady states. In another direction, the Mean First Passage Time of this process also is of profound importance since stochastic restarts may drastically reduce the expected run time of a computer algorithm, expedite the completion of a complex search process, or increase the rate of an enzymatic reaction. In particular, one of the diversities of the First Passage Times is its optimization. We carefully study a generic Stochastic Resetting process under a broad range of time dependent protocols and investigate its statistical properties. We further find the most general condition under which the Mean First Passage Time can be optimized among all restart strategies.

13. **Mechanism of Electrotunable Friction Measured in AFM Experiments with Ionic Liquids**

Karina Pivnic, Tel Aviv University, Israel

The interest in the molecular mechanisms of layering and friction of ionic liquids (IL) in electrified nanometer confinements has led to experimental force sensitive measurements employing atomic force microscope (AFM) [1-4]. Super-low friction (superlubricity) was demonstrated [3,4] to be switched on and off in situ, by polarizing the surface relative to the reference electrode, switching either to anion enriched or cation enriched layer. Using molecular dynamics simulations, we simulate a system mimicking such experiments. We focus on understanding a mechanism of electrotunable friction measured in AFM experiments when only one layer of IL is present between the surfaces. In particular, we investigate how does the orientation of the interfacial cation layer influences the friction and adhesion at such tribological contacts.

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14. **Analysis of Non-Markovian Effects in Enzymatic Catalysis**

Tsilil Rotbart, Tel Aviv University, Israel

Enzymatic reactions can be generally characterized by binding of a substrate molecule to an enzyme to form a complex which ultimately leads to the catalysis of the substrate to product and the unbinding of the complex to a product and a free enzyme which is free to start another cycle. These reactions have been well described by the Michaelis –Menten model for more than a century now. However, when one only examines enzyme catalysis in the bulk, many details of the inner mechanisms can be averaged in to very few measurable parameters. New experimental practices have opened the door to observing the catalysis of single enzyme molecules. These experiments, among other things, disputed an underlying assumption of the Michaelis-Menten model that the catalysis of substrate to product cannot be described as a memory-less process. In this work, we build a model which does not assume memory-less processes to describe the steps on the way to enzymatic catalysis and look in to the implication of such model. In particular we look at the non-trivial effect of increased unbinding rate between the substrate and the enzyme. Moreover, we expanded our model to include the interaction with inhibitors, and show what one might learn on the inner workings of the catalysis even in bulk experiments.

15. **Jamming vs. Caging in Three Dimensional Jamming Percolation**

Nimrod Segall, Tel Aviv University, Israel

We demonstrate that a three-dimensional kinetically-constrained model [1] exhibits two distinct phase transitions. The first – at a jamming density ρ_{ho_J} where there is a mixed-order phase transition in which a finite fraction of the particles become frozen in a directed-percolation manner, but other particles may still diffuse throughout the system. The second – at a caging density $\rho_{ho_C} > \rho_{ho_J}$, where mobile particles are trapped in finite cages and no longer diffuse. We develop a static analysis to infer on the dynamics of the system and show that the caging transition occurs due to percolation of the unfrozen sites. We show that it is a continuous transition with the same critical exponents as random percolation [2].

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16. ***Piece-wise Linear Elasticity***
Carmel Shor, Weizmann Institute of Science, Israel

It is already known that at zero temperature $T = 0$ the nonlinear coefficients do not exist and diverge in the thermodynamic limit. Later we will also show that this is the case also for finite temperature. Thus the question arise, how to explain the apparent non-linear behavior of the stress. We will show that in fact one should consider the elastic response of amorphous solids between plastic events, and there one can invariably define a piece-wise linear elastic response with shear modulus that is strain-dependent. This theory holds for low but finite temperatures, and gives an expression to calculate this strain-dependent shear-modulus. In order to support this theory, we performed numerical simulations of glasses using the Kob-Andersen model, in which point particles interact via a Lennard Jones potential. For each system size 100 samples were made, and then strained in finite temperature, letting the system to reach a steady-state after each strain increment (Thermal QuasiStatic TQS). The stress vs. strain curves were then analyzed, and it was shown that the true nature of the shear modulus can be faithfully explained with the piecewise strain dep. Modulus, without needing higher order coefficients. Furthermore, this approach can also explain the finite non-zero shear modulus appearing in the "steady-state regime" after the sample has yielded. The key ingredient in this analysis is the distinction between "quenched average", in which the shear modulus is calculated for each sample in the ensemble separately and then averaged, and "annealed average", in which all stress-strain curves were averaged, and then the slope was calculated. We show that the right way to look at the shear modulus is that of the quenched average.

17. ***Localization Due to Interaction-enhanced Disorder in Bosonic Systems***
Rajeev Singh, Bar-Ilan University, Israel

Localization in interacting systems caused by disorder, known as many-body localization (MBL), has attracted a lot of attention in recent years. Most systems studied in this context also show single particle localization and the question of MBL is whether the phenomena survives the effects of interactions. We consider a simple bosonic system with no single particle localization and show that interactions enhance the effects of very small disorder and result in localization when many particles are present. We provide physical insights into the mechanism involved and support our results with analytical and numerical calculations.

18. ***Relation Between Structure of Blocked Clusters and Relaxation Dynamics in Kinetically Constrained Models***
Eial Teomy, Tel Aviv University, Israel

In a liquid all the particles are mobile, while in a glass only some of them are mobile at any given time. Although overall the structure is amorphous in both cases, the difference is that in glasses there are local structures that inhibit the movement of particles inside them. We investigate these structures by considering the minimum number of particles that need to move before a specific particle can move. By mapping the dynamics of the particles to diffusion of mobile vacancies, we find a general algebraic relation between the mean size of the structures and the mean persistence time, which is the time until a particle moves for the first time. The exponent relating these two quantities depends on the system's properties. We investigated this relation analytically and numerically in several kinetically-constrained models: the Fredrickson-Andersen, Kob-Andersen and Spiral models. These models are either lattice gas models or Ising-like models, in which a particle can move or a spin can flip only if the local environment satisfies some model-dependent rule. Due the discrete nature of these models and relative simplicity, we were able to analytically find the relation between the structure and the dynamics and found an excellent agreement between our analytical results, our numerical simulations, and the heuristic arguments presented above. In these simple models, the minimum number of particles that need to move before a specific particle can move is easily found by using a culling algorithm, also called bootstrap or threshold percolation.

19. **Single DNA Molecular Rectifier Enabled By Structure Modification**
Elinor Zerah-Harush, Ben-Gurion University

The predictability, diversity and programmability of DNA make it a leading candidate for the design of functional electronic devices that use single molecules, yet its electron transport properties have not been fully elucidated. This is primarily because of a poor understanding of how the structure of DNA determines its electron transport. Here, DNA-based molecular rectifier is demonstrated constructed by site-specific intercalation of small molecules (coralyne) into a custom-designed 11-base-pair DNA duplex. Measured current–voltage curves of the DNA–coralyne molecular junction show unexpectedly large rectification with a rectification ratio of about 15 at 1.1 V, a counter-intuitive finding considering the seemingly symmetrical molecular structure of the junction. A non-equilibrium Green’s function-based model— parameterized by density functional theory calculations—revealed that the coralyne-induced spatial asymmetry in the electron state distribution caused the observed rectification. This inherent asymmetry leads to changes in the coupling of the molecular HOMO⁻¹ level to the electrodes when an external voltage is applied, resulting in an asymmetric change in transmission

Cunlan Guo, Kun Wang, Elinor Zerah-Harush, Joseph Hamill, Bin Wang, Yonatan Dubi, Bingqian Xu. Molecular rectifier composed of DNA with high rectification ratio enabled by intercalation. Nature Chemistry 8, 484–490 (2016).