



2016 非平衡态热力学和统计物理理论及其应用 学术研讨会

北京大学
2016 年 11 月 26-27 日





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会议地点:

北京国际数学研究中心, 镜春园82甲乙丙楼二楼报告厅, 北京大学

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会议邀请报告人:

1. 敖 平, 上海交通大学
2. 陈晓松, 中科院理论物理研究所
3. 葛 颀, 北京大学
4. 蒋达权, 北京大学
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12. 涂展春, 北京师范大学
13. 赵 鸿, 厦门大学





- 14. 郑波, 浙江大学
- 15. 郑志刚, 华侨大学
- 16. 钟凡, 中山大学
- 17. 周海军, 中科院理论物理研究所
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日程安排

11月26日上午

主持人: 敖平		
8:45-9:00		开幕式, 合影
9:00-9:30	欧阳颀	生物能量系统中的能量分配
9:30-10:00	陈晓松	Criticality and Universality classes of d-dimensional lattice networks with long-range connections
10:00-10:30	郑波	Landau-Lifshitz-Gilbert equation and phase transitions
10:30-11:00	Break	



主持人：郑波		
11:00-11:30	郑志刚	Interface Facilitated Energy Transport in Coupled Nonlinear Lattices
11:30-12:00	钟凡	Theory of Driven Nonequilibrium Critical Phenomena
12:00-13:30	午餐 畅春园	

11月26日下午

主持人：欧阳颢		
14:00-14:30	敖平	Dynamical relations in nonequilibrium processes
14:30-15:00	汤雷翰	Energy dissipation in time-scale separated Markov systems
15:00-15:30	蒋达权	Nonequilibrium fluctuations of some Markov systems
15:30-16:00	Break	
主持人：汤雷翰		
16:00-16:30	赵鸿	布朗运动的完全解
16:30-17:00	柳飞	Quantum Feynman-Kac formula
17:00-17:30	全海涛	Stochastic Thermodynamics of a Particle in a Box
17:30-18:00	葛颢	Nonequilibrium thermodynamics of stochastic chemical reaction systems

11月27日上午

主持人：赵鸿		
9:00-9:30	周海军	Cycles and feedback interactions in directed biological networks
9:30-10:00	涂展春	等温捷径
10:00-10:30	Break	



主持人：涂展春		
10:30-11:00	兰岳恒	Identification of Bacterial community with Legendre expansion
11:00-11:30	童培庆	TBD
11:30-12:00	周昕	Effectively explore metastable states of proteins by adaptive non-equilibrium driving simulations
12:00-13:30	午餐 畅春园	

题目和摘要

题目：Dynamical relations in nonequilibrium processes

报告人：敖平(上海交通大学)

摘要：Within last 2 decades there have been un-anticipated important progresses in nonequilibrium processes. One of them is the free energy equality or Jarzynski equality, in which the difference in stationary state free energy can be found by a dynamical measurement. While such equality is powerful, it leaves the real dynamical structure untouched by the implied assumption of pre-existence of "hamiltonian". My lab has been focusing on dynamical side of the problem. Here I would like to discuss the generic dynamical structure for nonequilibrium processes and other types of stochastic dynamical equalities, such as the generalized Einstein relation (GER). In particular, I will reason that GER and free energy equality are two sides of same process. The experimental implications will also be discussed.

题目：Nonequilibrium thermodynamics of stochastic chemical reaction systems

报告人：葛颢(北京大学)

摘要: Nonequilibrium thermodynamics and statistical physics in terms of stochastic models entered a stage of vigorous development since 1970s, which well fit the development of advanced experimental techniques in modern physical chemistry and biochemistry. I will discuss our recent stochastic approaches to investigate the nonequilibrium thermodynamics of chemical reaction systems. We show that the entropy production rate can be decomposed into the housekeeping heat and the decreasing rate of relative entropy, both of which are nonnegative, followed by a more stronger version of Clausius inequality. We further proved that in the macroscopic limit by merely allowing the molecular numbers to infinite, a generalized macroscopic free energy and its balance equation emerge. The balance equation is valid generally in isothermal driven systems. A general fluctuation dissipation theorem for stochastic reaction kinetics is also proved. Such an emergent "law" is independent of underlying kinetic details. The mathematical theory illustrates how a novel macroscopic dynamic law can emerge from the mesoscopic kinetics in a multi-scale system.





题目：Nonequilibrium fluctuations of some Markov systems

报告人：蒋达权(北京大学)

摘要: Markov chains and diffusion processes are widely used to model various stochastic systems in physics, chemistry, biology, etc. In this talk, we will present some fluctuation properties of nonequilibrium systems modelled by such Markov processes.

More concretely, owing to a newly discovered symmetry of Brownian motion named as the quasi-time-reversal invariance, we prove an equality for diffusion processes on the circle named as the cycle symmetry, which says that the distributions of the forming times of the forward and backward cycles, conditioned on that the corresponding cycle is formed earlier than the other, are exactly the same. We show that the cycle symmetry leads to the large deviation principle of the sample circulations of diffusion processes on the circle, in which the rate function has a highly non-obvious symmetry. Further extensions and applications are also discussed, especially the fluctuation theorems for the sample net circulation and the sample entropy production rate. Similar results hold for recurrent Markov chains with denumerable states.

For inhomogeneous continuous-time Markov chains, we prove rigorously three types of fluctuation-dissipation theorems (FDTs), thus extend the previously derived FDTs to the inhomogeneous case. Further physical and biochemical applications are also discussed.

题目：Identification of Bacterial community with Legendre expansion

报告人：兰岳恒(北京邮电大学)

摘要: With the rapid development of biotechnology, it becomes possible to identify the identity and proportion of bacteria in a bio-sample through an assay of nucleotide sequency. One such technique is by checking the 16RNAs segment of the bacterial RNA. The multiple sequence alignment method is accurate but way too slow and several more efficient methods are proposed based on the k-mer statistics. Here, we propose an alternativeway to extract the information content embedded in the RNA sequence based on the Legendre expansion which is proved to be very efficient while retaining considerable accuracy.

题目：Quantum Feynman-Kac formula

报告人：柳飞(北京航空航天大学)

摘要: Feynman-Kac (FK) 公式是经典随机过程的一个著名公式。它把偏微分方程和随机过程紧密地联系在一起。近期, FK 公式又在非平衡理论中得到了新的应用: 它为非平衡功等式的证明和功分布的计算提供了一个相当有效的方法。那么在量子非平衡过程中, 是否也有量子版本的 FK 公式? 在本报告中, 我将指出, 对于两类特殊的过程, 包括封闭的量子系统和马尔科夫量子主方程, 我们的确可以模仿经典方法, 形式地得到量子 FK 公式。根据量子-经典对应原理, 当普朗克常数趋于零时, 这个公式退化成经典版本。即使如此, 我们还必须面对量子 FK 公式是否真的物理相关的问题, 比如是否和量子的功有关? 如果是, 能否应用于功分布的计算? 我们发现, 只有引入两次能量投影测量和量子跳跃轨迹的概念, 这些问题才能够得到肯定的回答。

题目：生物能量系统中的能量分配





报告人：欧阳颀(北京大学)

摘要：生物功能和非平衡态热力学之间的关系成为近年来研究非常活跃的领域。传统观点中生物系统主要是将能量用于一些物理或化学过程。最近关于动态校验[1]和生物适应性[2]和生物振荡[3]的研究表明，有功能的生物网络必须具有群体协同性，该功能的执行与能量消耗高度相关。本报告主要讨论生物节律协同性的热力学问题。生物振荡是一个典型的生命过程，包括细胞周期，生物节律，以及在合成生物学中的可振荡基因调控网络。这些网络都工作在细胞尺度的体积内，相关分子数目在百量级。单细胞水平的动力学会受到环境和小分子数目两方面带来的涨落。我们关心的是，这些系统如何在涨落的环境中保持群体有序的振荡行为，保持这种有序性的能量代价，以及物理化学过程与信息交流过程之间的能量分配。我们系统考察了蓝藻菌中 Kai 系统的振荡行为。我们发现，能量的耗散主要用于蛋白质建的信息交流，以此来抑制相位的扩散和维持振荡的群体时间有序性。

参考文献：

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- [2]. Lan, G., et al., The energy-speed-accuracy tradeoff in sensory adaptation. *Nat Phys*, 2012. 8(5): p. 422-428.
- [3] Y.S. Chao, H.L. Wang, Qi Ouyang and Y.H. Tu, *The free energy cost of accurate biochemical oscillations*, *Nature Physics*, 11, (2015), 772–778.

题目：Stochastic Thermodynamics of a Particle in a Box

报告人：全海涛(北京大学)

摘要: The piston system (particles in a box) is the simplest paradigmatic model in traditional thermodynamics. However, the recently established framework of stochastic thermodynamics (ST) fails to apply to this model system due to the embedded singularity in the potential. In this Letter, we study the ST of a particle in a box by adopting a novel coordinate transformation technique. Through comparing with the exact solution of a breathing harmonic oscillator, we obtain analytical results of work distribution for an arbitrary protocol in the linear response regime and verify various predictions of the fluctuation-dissipation relation. When applying to the Brownian Szilard engine model, we obtain the optimal protocol $\lambda_t = \lambda_0 2^{t/\tau}$ for a given sufficiently long total time τ . Our study not only establishes a paradigm for studying ST of a particle in a box but also bridges the long-standing gap in the development of ST.

题目：等温捷径

报告人：涂展春(北京师范大学)

在有限时间内连接具有相同温度的两个平衡态的策略称为等温捷径。对于一个与恒温热浴接触的系统，引入一个辅助的场使得扩展系统的分布函数沿着原始系统的即时正则分布演化，当限制初始和终了时刻的辅助场为零，就可以获得等温捷径。基于随机热力学和等温捷径，我们证明了三个非平衡等式：(1) 首末状态的自由能差刚好等于原始系统势能改变做的功；(2) 等温捷径过程中的耗散功与过程持续的时间成反比；(3) 广义 Jarzynski 等式，其形式与 Jarzynski 等式相同，但是可以从任意初始态出发。数值计算验证了三个非平衡等式的可靠性。





题目：布朗运动的完全解

报告人：赵鸿(厦门大学)

摘要：Einstein 1905 年给出了布朗运动的物理描述,随后 Uhlenbeck (1930)等发展了刻画其运动的 kinetics (分子运动论),然而 1970 年左右的研究发现 kinetics 理论并不准确,布朗粒子的运动还具有记忆效应,表现为速度自关联函数随时间幂率衰减而不是 kinetics 理论预言的指数衰减. 迄今为止,虽然提出了一系列的理论和公式,但是对布朗运动的全面统一的理论还远没有完成.

近十几年来,实验技术的发展使得直接测量布朗粒子的即时速度和位置成为可能,从而 nature,science 等杂志上出现了大量的实验研究工作,探测布朗粒子运动的记忆效应也就是流体力学效应是这些工作的目标之一. 因此,完善布朗粒子运动理论不仅具有理论价值而且具有现实意义. 本报告将报告我们近几年来在布朗运动理论方面的进展,给出一般性的描述自关联函数和扩散系数的解析公式.

题目：Landau-Lifshitz-Gilbert equation and phase transitions

报告人：郑波(浙江大学)

摘要: We numerically solve the Landau-Lifshitz-Gilbert equation, and investigate the non-equilibrium dynamic behavior of phase transitions, including the pinning-depinning phase transition and order-disorder phase transition. For the first time, the transition temperature and critical exponents are quantitatively determined.

题目：Interface Facilitated Energy Transport in Coupled Nonlinear Lattices

报告人：郑志刚(华侨大学)

摘要：It is generally expected that the interface coupling leads to the suppression of thermal transport through coupled nanostructures due to the additional interface phonon-phonon scattering. However, recent experiments demonstrated that the interface van der Waals interactions can significantly enhance the thermal transfer of bonding boron nanoribbons compared to a single freestanding nanoribbon. To obtain a more indepth understanding on the important role of the nonlinear interface coupling in the heat transports, we explore the effect of nonlinearity in the interface interaction on the phonon transport by studying the coupled one-dimensional (1D) Frenkel-Kontorova lattices. It is found that thermal conductivity increases with increasing interface nonlinear intensity for weak interchain nonlinearity. By developing the effective phonon theory of coupled systems, we calculate the dependence of heat conductivity on interfacial nonlinearity in weak interchain couplings regime which is qualitatively in good agreement with the result obtained from molecular dynamics simulations. Moreover, we demonstrate that, with increasing interface nonlinear intensity, the system dimensionless nonlinearity strength is reduced, which in turn gives rise to the enhancement of thermal conductivity. Our results pave the way for manipulating the energy transport through coupled nanostructures for future emerging applications.





题目 : Theory of Driven Nonequilibrium Critical Phenomena

报告人 : 钟凡(中山大学)

摘要 : A system driven in the vicinity of its critical point by varying a relevant field in an arbitrary function of time is a generic system that possesses a long relaxation time compared with the driving time scale and thus represents a large class of nonequilibrium systems. For such a manifestly nonlinear nonequilibrium strongly fluctuating system, we shall show that there exists universal nonequilibrium critical behavior that is incredibly well described by its equilibrium critical properties. A dynamic renormalization-group theory is developed to account for the behavior. We shall show that the weak driving may give rise to several time scales depending on its form and thus rich nonequilibrium phenomena of various regimes and their crossovers, negative susceptibilities, as well as a violation of fluctuation-dissipation theorem and hysteresis. An initial condition that can be in either equilibrium or nonequilibrium but has longer correlations than the driving scales also results in a unique regime. The implication of the results on measurement will also be discussed.

题目 : Cycles and feedback interactions in directed biological networks

报告人 : 周海军(中国科学院)

摘要 : Many biological networks, such as neural networks and gene transcription networks, are directed networks. A strongly connected component of such a network often contains a lot of directed cycles. Such cycles make the non-equilibrium dynamical property of the system difficult to study. In this presentation I will discuss the important issue of distinguishing feedforward and feedback interactions in directed networks, and present a method to quantify the degree of intrinsic directness of a network. Our work builds on "the principle of minimum-feedback" advocated by Yueheng Lan and co-workers. Our work might be helpful in identifying the most significant arcs for feedback interactions.

题目 : Effectively explore metastable states of proteins by adaptive non-equilibrium driving simulations

报告人 : 周昕(中科院大学)

摘要 : Non-equilibrium drivings applied in molecular dynamics (MD) simulations can efficiently improve visiting efficiency in conformational regions of proteins, but not suitable drivings might make the systems go too far away from equilibrium thus mainly explore irrelevant conformations. So far, ones often have to empirically preset smaller drivings to avoid the accumulation of non-equilibrium effects. Here we proposed a method, named as adaptive non-equilibrium simulations (ANES), to automatically adjust the external driving on the fly, based on a feedback to the short-time average response of system. The ANES approximately keeps the local equilibrium inside each of metastable states but accelerates the slow transitions among these states and varies the interstate equilibrium. Thus, the method can focus on stable and metastable protein conformations while it significantly accelerates the transitions among states. We illustrated the application of the





ANES in a peptide, deca-alanine and in a small protein, HP35, to show its ability in high efficiently exploring metastable conformations of proteins.

