N 统计物理与复杂体系

分会召集人：汤雷翰、郑波、周海军、赵鸿

N01

专题代号：N

量子隧穿与强场电离与激光聚变

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摘要：

本报告对量子隧穿及其拓展概念进行了评述，特别讨论了量子隧穿发生的温度空间标度及其所需时间问题。之后讨论了强场电离及激光聚变中的隧穿问题并汇报了最新研究进展。

N02

专题代号：N

界面声子/热输运：一维原子链模型

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摘要：

本报告将介绍我们在界面声子/热输运方面的一些研究进展。 基于一维的原子链模型， 我们先后发现了最大界面热导（最佳界面耦合常数）、非线性增强热导、以及最佳界面耦合材料。 最近我们发现，通过调节界面材料参数，可以有效提高界面热导， 几何梯度材料是理想的热传导界面材料。我们发现的手性声子是最近的一个研究热点， 进一步研究发现界面可以有效调节声子手性， 并发现了界面处声子的四分之一波倍数的损失。

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N03

专题代号：N

亚稳态，声子寿命的双标度行为和契里克夫非线性共振

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摘要：

Phonon lifetime is an important quantity to understand the phonon-phonon interaction and corresponding thermal transport. Equipartition and thermalization in complex dynamical systems are cornerstone concepts to explore the fundamental of statistical mechanics. In this talk, I will brief review our recent studies on thermal transport and present an analytical approach to quantify the energy of phonon modes of low-dimensional nonlinear systems. Via the approach the phonon lifetime could be measured and the dynamical thermalization has been studied. In particular, we found the existence of the metastable state of theφ^4 system in small nonlinearity regime. With the increase of nonlinearity, thermalization time decreases firstly in a power-law behavior and anomalously increases in the regime of large nonlinearity, which comes from the existence of discrete breather. Meanwhile, a bi-scaling behavior of phonon lifetime is observed, which can be understood by Chirikov nonlinear resonance.

关键词：Phonon lifetime; dynamical thermalization; metastable state; Chirikov nonlinear resonance

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N04

专题代号：N

Nonintegrability and Thermalization of One-dimensional Lattices

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Abstract: Nonintegrability is a necessary condition for the thermalization of a generic Hamiltonian system【1】. In practice, the integrability can be broken in various ways. As illustrating examples, we numerically studied the thermalization behaviors of two types of one-dimensional (1D) diatomic chains in the thermodynamic limit. One chain was the diatomic Toda chain whose nonintegrability was introduced by unequal masses. The other chain was the diatomic Fermi-Pasta-Ulam-Tsingou-β chain whose nonintegrability was introduced by quartic nonlinear interaction. We found that these two different methods of destroying the integrability led to qualitatively different routes to thermalization, but the thermalization time, T_{eq}, followed the same law; T_{eq} was inversely proportional to the square of the perturbation strength. This law also agreed with the existing results of 1D monatomic lattices【2,3】. All these results imply that there is a universal law of thermalization that is independent of the method of breaking integrability 【4】.

Key words： Nonintegrability, thermalization, one-dimensional lattice

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N05

专题代号:N

Quantum Severalty: Speed up versus Suppresion

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Protein folding is an important topic in the interdisciplinary field involving molecular biology, computer science as well as theoretical physics, in which the Levinthal paradox has long been a standing theoretical question. Previous progresses, till now, are made on the base of energy-landscape with various artificial hypotheses. This just likes the case, if one stays on the classical picture of planetary model of atoms to interpret the atomic line-shaped spectra, the so-called Bohr-Summerfield quantization condition must be imposed as a hypothesis. Recently, we introduced a self-contained quantum approach to investigate the protein folding problem without artificial hypotheses, modeling protein as quantum walks on definite graphs.

After a brief introduction of both the scientific and academic background, I will describe the key points of our quantum theory for a fast protein-folding time. Then I present our consideration for the model with more amino-acids residues where more concepts such as compactness and distance-space projections are introduced. Our investigation reveals the existence of quantum intelligence hidden behind in the protein folding pathways. Furthermore, we abbreviate to a float-vertex graph model, and find a quantum severalty –speed up and suppress effect.

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N06

专题代号:N

量子孤立系统之平衡态概念的微观动力学基础——现状与展望

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孤立系统的平衡态概念，在热力学与统计物理中具有核心重要性。然而，其微观动力学基础迄今尚未完全清楚，而厘清该基础是众多研究工作的目标。首先，我们简介近十多年来热化领域中的一些重要进展。然后，在一个适当的框架之中，提议一个实现上述目标的技术路线。最后，结合我们近年来在量子混沌与半扰动论方面的成果，讨论实施该路线所已经拥有的技术准备，并展望未来所需解决的问题。

关键词：量子孤立系统，热化，平衡态，量子混沌，半扰动论。

N07

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Concentration-measure theory of waves: new perspectives of the fundamentals of nonequilibrium statistical physics and mesoscopic physics

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Abstract: The foundations of statistical physics are currently under renovations. A number of scenarios for the arising of statistical physics in an individual system has been proposed. However, most studies have focused on equilibrium statistical physics. In this talk, I shall report our recent progress on the fundamentals of nonequilibrium statistical physics. I will show a theory for structures and fluctuations of waves in individual disordered media, using the mathematical tool of the concentration of measure. Applying this theory, we can see how the elementary nonequilibrium process of diffusion can arise from a single scattering state of wave equation, without the canonical hypothesis of ensembles. Furthermore, fluctuations associated with the change in incoming waves exhibit a new kind of universalities, which does not exist in conventional mesoscopic fluctuations associated with the change in disorder realizations, and originate from the coherence between the natural channels of waves – the transmission eigenchannels.

Key words: nonequilibrium statistical physics, mesoscopic physics, disordered media, concentration of measure, transmission eigenchannels

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N08

专题代号:N

固液界面预熔化相变耦合的液滴浸润与铺展

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摘要：我们应用分子动力学模拟方法研究了液相金属 Pb 液滴在 Al 金属(111)表面上非平衡态铺展动力学与平衡态浸润行为。我们曾在接近 Al 熔点温度区间发现了 Al-Pb 固液界面中的预熔化相变现象[Phys. Rev. Lett, 110, 096102 (2013)]，而Al(111)表面无法表面熔化，我们发现 Pb 液滴在 Al 金属(111)光滑表面上的非平衡态铺展过程同时伴随着界面结构相变。我们研究了液滴铺展与固液界面预熔化的耦合机制，并将分子模拟测量的液滴铺展动力学结果与两种非平衡态铺展动力学理论模型进行了定量比较。两种铺展理论模型包括：1）流体力学铺展模型—铺展能量耗散由粘性弛豫主导；2）动力学铺展模型—铺展能量耗散由界面摩擦主导。这两种铺展模型对于液滴半径的时间依赖关系分别给出不同的幂次定律。在预熔化相变发生的温度区间（875K 到 922.4K），液滴铺展遵循动力学铺展模型的理论预言。在较低温度 625K（铅凝固点以上）固液界面没有出现预熔化相变并为光滑界面结构的情况下，液滴铺展遵循流体力学铺展模型的理论预言。当液滴在附加简谐弹性约束到 Al 表面原子以限制固液界面预熔化相变的 Al(111)表面上铺展时，我们观察到铺展仍遵循动力学铺展模型的理论预言，但最终获得平衡态浸润接触角相较于同样温度下有预熔化相变发生的体系有了大幅提升。于是，我们得出结论，固液界面预熔化相变的出现强烈影响到 Al(111)/Pb 固液界面的热力学性质，但对铺展动力学机制的影响很小。最后，我们还发现了在固液界面预熔化相变发生时液滴接触线呈现出双接触角共存的特殊结构，与反应浸润体系的接触线结构相似。

关键词：液滴、浸润、铺展动力学、预熔化相变、分子动力学模拟

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N09

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Nonplanar Whirling Motions in Carbon Nanotubes Resonators

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In recent years, the nonlinear dynamics of carbon nanotubes has drawn much attention of scientists/researchers due to its unique mechanical properties and significant application potentials ranging from ultrasensitive mass sensor to single-electron spin detection. In this work, the nonlinear and chaotic motions of the single wall carbon nanotubes (SWCNT) subjected to an external driven force are investigated with extensive molecular dynamics (MD) simulations. The SWCNT has a length of L=30nm, and is assumed to clamped at both ends, with the next four layers being taken as thermostat atoms and the remaining are treated as Newtonian atoms. After the initial relaxation, a uniform driven force is applied to the SWCNT, and the trajectory of the center of the SWCNT is used to investigate the dynamical behavior of the system. The numerical results show that, for the small driven force, the dynamics appear to be linear and the SWCNT oscillates within a fixed plane. However, as the driven force is sufficiently large to yield substantial bending and consequently strong axial stress, the planar motion is no longer stable and a whirling or “jump-rope” like motion occurs due to the nonlinear interaction between orthogonal vibrational modes, which is consistent with the previous theoretical results [1, 2]. Furthermore, rich dynamical behaviors have been identified towards the development of chaos and the transition between different types of chaotic motions.

Keyword：Carbon Nanotubes, Molecular Dynamics Simulations, Nonplanar Whirling Motions

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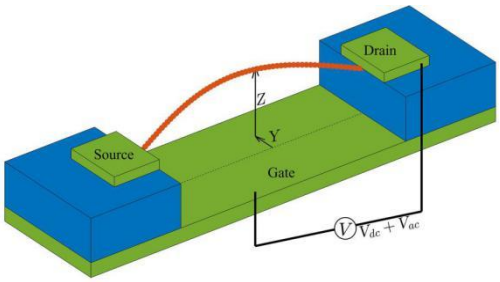

N10

专题代号:N

包含奇偶控制参数的随机热力学

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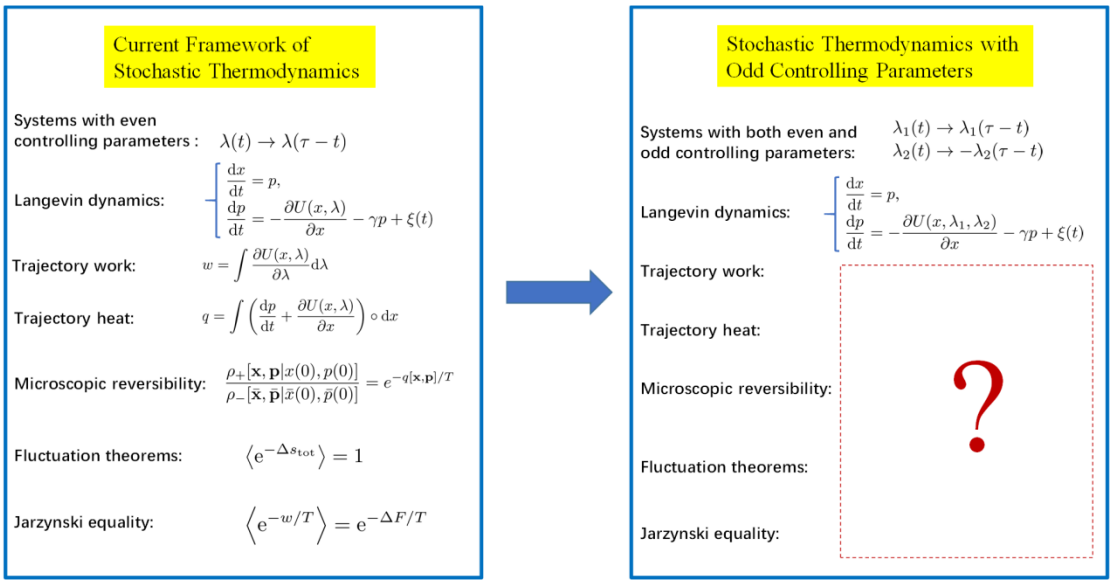
摘要：当受控的小系统既包含奇控制参数（即在时间反演下变号），又包含偶控制参数（即在时间反演下不变号）时，传统随机热力学框架中轨迹热的定义与微观可逆性条件是不相容的。需要我们将传统随机热力学框架拓展到包含奇控制参数的情形。通过引入伴随动力学，我们将总熵产生分解为三部分，其中两部分满足涨落定理的形式。通过修改微观可逆性条件，我们导出了几个非平衡功关系式，包含类 Jarzynski 等式、类 Crooks 功关系式。

关键词：随机热力学，奇参数，熵产生，非平衡功关系式



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N11

专题代号:N

Statistics of entropy production infima in an asymmetric granular motor

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Abstract: The total entropy for an isolated system will on average not decrease, but the entropy's increment is not smooth due to intrinsic fluctuations in the system. Recently there is a theoretical work stating that the mean of the finite-time infimum of the stochastic entropy production is bounded by minus the Boltzmann constant. Here we investigate the entropy production process in an asymmetric granular motor, where fluctuation dominates the system. It is found that under certain conditions, the system can be described by the Langevin equation well and satisfies the fluctuation theorem. We will discuss the parameter ranges in the experiment that when the description of the Langevin equation is valid, and demonstrate that in this case, the mean of the entropy production infima is indeed bounded by minus the Boltzmann constant, although due to finite length of the data, fluctuations may exceed that bound.

Keywords: entropy production, finite-time infimum, granular motor

N12

专题代号:N

Equilibrium and non-equilibrium dynamics in the behavior of bacterial flagellar motor

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摘要：Flagellated bacteria swim by rotation of the helical flagellar filaments, each driven at its base by a reversible rotary motor – the bacterial flagellar motor. Rotation direction of the motor (clockwise or counter clockwise) determines the swimming modes (run or tumble) of the bacteria. The behavior of the bacterial flagellar motor exhibits rich equilibrium and non-equilibrium dynamics, two examples of which will be presented in this talk: non-equilibrium dynamics in the allosteric regulation of the bacterial flagellar switch; equilibrium dynamics in the turnover of the torque-generating units (stators).

关键词：allosteric regulation, adaptive remodeling.

基金项目：国家自然科学基金项目（NO. 11374282, 21573214, and 11872358）

N13

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位错相互作用对晶界结构的影响

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位错和位错扩散决定了晶体的力学性质及其对外力的响应特性。了解位错的运动特点及位错间相互作用，对控制和消除位错缺陷，提高晶体的力学和光电性质有深远意义。利用二维胶体晶体，我们研究了位错在晶体生长过程中的扩散，及位错间的反射、融合与湮灭等过程，揭示了晶体对称性与位错运动和晶界结构间的物理关联，为全面理解位错的物理性质、控制缺陷、提高晶体物理特性提供了新的物理认识。

关键词：晶体 位错 晶界

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N14

专题代号:N

Breathing Cluster in Networked Chaotic Oscillators

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摘要：A new phenomenon, namely breathing synchronization cluster, is observed in complex network of coupled chaotic oscillators. In specific, it is found that a fraction of the oscillators in a large-size complex network may form a synchronization cluster and, as the system evolves, the cluster could be switching alternatively between the synchronization and desynchronization states. In the meantime, the other oscillators in the network are always in the desynchronization states. We demonstrate this intriguing phenomenon in different network models and conduct a theoretical analysis on the underlying mechanism. Finally, the implications of breathing cluster to brain functions, e.g., memory and sleep, will be discussed.

关键词：Complex network, Cluster synchronization, Pattern formation

N15

专题代号：N：统计物理与复杂体系

Hydrodynamic and entropic effects on colloidal diffusion in corrugated channels

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Abstract： When a particle diffuses in a corrugated channel, the channel's boundaries have a twofold effect of limiting the configuration space accessible to the particle and increasing its hydrodynamic drag. Analytical and numerical approaches well-reproduce the former (entropic) effect, while ignoring the latter (hydrodynamic) effect. Here, we experimentally investigate nonadvective colloidal diffusion in channels with periodically varying width. While validating the current theory for channels much wider than the particle radius, we show that, in narrow channels, hydrodynamic and entropic effects can be equally strong and that hydrodynamic effects can be incorporated into existing descriptions by using an experimentally measured diffusivity. These results significantly advance our understanding of diffusive transport in confined geometries, such as in ionic channels and nanopores.

Key Words： diffusion; colloid; confinement; hydrodynamics; entropic effects

N16

专题代号:N

基于复杂网络方法的时间序列分析

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非线性时间序列分析的主要目的在于揭示实际数据隐含的内在动力学特性及系统复杂性现象。这些数据包罗万象，比如人脑神经系统电生理活动数据：心电（ECG）、脑电（EEG）、神经电活动、大脑活动成像数据（CT、核磁共振成像、近红外光谱成像）等；地球物理领域内和气候变化相关的气象观测数据：地表温度、海表温度、风向和气压等；人类社会活动中的经济数据：股票交易、个人网购交易数据等。以非线性动力学理论为基础的通常做法是：对于给定的一个时间序列，首先通过时间延迟嵌入方法，在相空间内重构出与内在动力系统拓扑等价的吸引子。基于重构的吸引子，可以从两个方面去揭示系统是否存在混沌等非线性动力学的基本特性。(i) 动态方面，如通过计算李雅普诺夫指数或熵获得；(ii) 几何方面，如通过分形维数或关联维数等指标刻画。这些常用物理量相互联系和补充，从不同的角度勾画非线性系统的动力学行为。

把非线性动力学理论和复杂网络理论相结合，从复杂网络的角度进行非线性时间序列分析是本领域的一个重要前沿热点之一。本文将回顾近十年来常用的方法，着重强调转换方法的研究进展，揭示其在识别系统耦合方向和大脑功能网络构建等两个方面的重要应用。

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N17

专题代号:N

A General Deep Learning Framework for Network Reconstruction and Dynamics Learning

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Abstract
Many complex processes can be viewed as dynamical systems on networks. However, in real cases, only the performances of the system are known, the network structure and the dynamical rules are not observed. Therefore, recovering latent network structure and dynamics from observed time series data are important tasks because it may help us to open the black box, and even to build up the model of a complex system automatically. Although this problem hosts a wealth of potential applications in biology, earth science, and epidemics etc., conventional methods have limitations. In this work, we introduce a new framework, Gumbel Graph Network (GGN), which is a model-free, data-driven deep learning framework to accomplish the reconstruction of both network connections and the dynamics on it. Our model consists of two jointly trained parts: a network generator that generating a discrete network with the Gumbel Softmax technique; and a dynamics learner that utilizing the generated network and one-step trajectory value to predict the states in future steps. We exhibit the universality of our framework on different kinds of time-series data: with the same structure, our model can be trained to accurately recover the network structure and predict future states on continuous, discrete, and binary dynamics, and outperforms competing network reconstruction methods.
Keywords: Network reconstruction; Dynamics learning; Graph network

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N18

专题代号：N

过冷液体中的局域连接度与动力学反常输运行为

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摘要：玻璃形成液体的动力学行为一直是物理、化学、生物、和材料等诸多研究领域的热点问题之一，到目前为止，人们并没有良好的理论框架和范式来理解和描述玻璃形成液体及玻璃态物质中的诸多异常行为。 玻璃形成液体具有诸多简单液体所不具备的动力学特征，比如系统的非自然指数性弛豫行为和结构弛豫时间的强温度关联性。非自然指数形式的时间关联函数也通常被认为是玻璃液体的典型特征之一。当对过冷液体进行淬火时，随着温度的降低系统逐渐偏离平衡态，此时系统的时间关联函数会从拉伸自然指数衰减（stretched exponential decay）形式逐步转变为压缩自然指数衰减（compressed exponentials），玻璃态中后一种形式的衰减常常被认为与体系内部的内应力释放有关，但其微观机制确有待于进一步的考察。非晶物理的研究经验告诉我们，玻璃形成体系的任何物理性质一般都是温度的平滑函数，所以上述这种在玻璃转变点左右到弛豫方式到转换并不太可能由一些未知隐参量的突然跳变产生。因此，压缩自然指数衰减的弛豫方式极有可能已存在于降温过程中的玻璃形成液体当中，此次的研究工作证实了这一之前未报道过的预想。在一种典型的金属玻璃形成液体（CuZr 系统）当中，研究发现拉伸和压缩自然指数衰减所对应的两种结构弛豫模式可以在玻璃转变温度以上共存，并可直接跟某些特定的结构单元进行关联。这一结果表明，深过冷液体中原子的动力学行为异常复杂，相互作用、相互影响下的输运方式丰富多彩，提示人们要尝试从多空间尺度和具有非局域性质的结构序参量上来理解和研究复杂液体的动力学行为。与此同时，本次工作也为研究金属玻璃所展现出的优良力学性质提供了新的思路和认识角度。

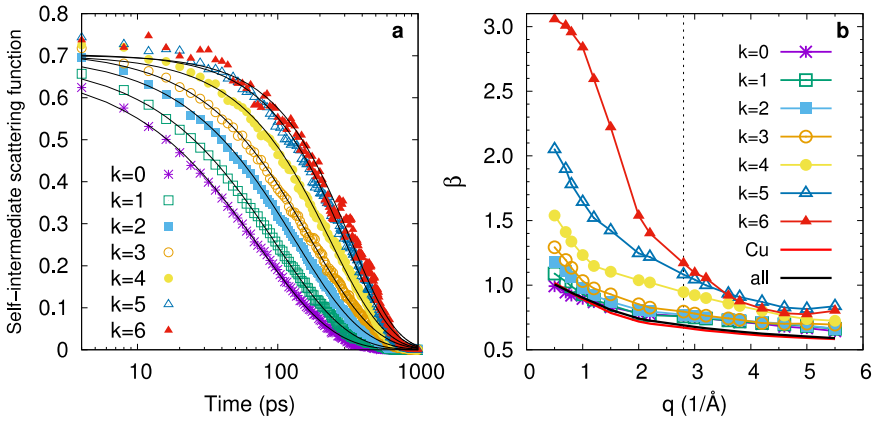

图 1 过冷液体的动力学弛豫函数和反常输运行为

关键词：过冷液体 弛豫函数 反常输运 分子动力学模拟

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N19

专题代号：N

Cluster mean-field dynamics in one-dimensional TASEP with inner interactions and Langmuir dynamics

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Abstract: In the area of statistical physics, totally asymmetric simple exclusion process (TASEP) is treated as one of the most important driven-diffusive systems. It contains profound non-equilibrium statistical physics mechanisms due to being the paradigm model like Ising model. Different with previous work, a one-dimensional TASEP coupled with inner interactions and Langmuir dynamics is taken into account. Weak coupled binding and unbinding rates are introduced in the proposed model. Bond breaking and making mechanisms of self-driven particles illustrating the unidirectional movement of protein motors are investigated by means of performing cluster mean-field analyses. Dynamics in the proposed system dominated by the competition between the attraction effect and the repulsion one are found to depend on the specific value of the interaction energy of these active particles. The research work will be helpful for understanding non-equilibrium statistical behaviors of interacting particle systems.

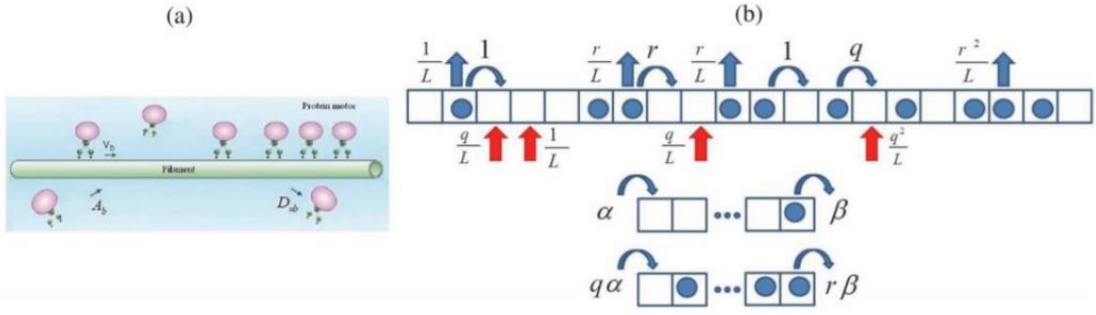

Fig. 1. The sketch of the model. (a) Intuitive illustrations depicting the motion of protein motors and (b) random-sequential update rule of the proposed system including bulk and boundaries. Arrows show allowed motions.

Keywords: TASEP; cluster mean-field analysis; inner interactions; Langmuir dynamics

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N20

专题代号:N

相分离过程的离散玻尔兹曼建模与模拟研究进展

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相分离是统计物理与软物质领域的重要研究课题。在单介质相分离研究中，我们习惯将密度高的相称为液相，而把密度低的相称为气相。这样，我们便可以借助多相流领域的理论和研究成果来理解软物质系统中的相分离行为。传统流体动力学方法往往基于经验、唯像、线性本构，主要关注密度、动量和能量（分布函数的守恒矩）及其演化；而研究表明，流体界面的精细物理结构与具体非平衡行为特征处理的得当与否直接影响着密度、温度、流速、压强等宏观行为描述的准确程度。基于动理学理论的离散 Boltzmann 方法（DBM）部分继承了 Boltzmann 方程的跨尺度物理描述能力，能够更加方便给出宏观行为特征更准确描述所需的最必要精细物理结构和具体非平衡特征。

本报告介绍离散 Boltzmann 方法（DBM）及其在相分离领域的应用。主要内容包括：（1）给出多相流系统中熵产生速率与非平衡特征量之间的关系、系统演化过程中引起熵增的主要机制及其相对的重要性；（2）发现非平衡强度和熵产生速率在相分离的第一阶段（亚稳相分解，SD）都随时间增加，而在第二阶段（相畴增长，DG）都随时间降低，非平衡强度和熵产生速率极大值点都可以作为划分相分离过程两个阶段新的物理判据；（3）相分离过程中热流、粘性和表面张力对于相分离第一阶段的持续时间、非平衡强度和熵产生特性的影响，对比流场中的宏观量和形态学特征量给出合理的物理解释；（4）分析相分离过程中不同非平衡行为之间、两种熵产生机制之间的关联、协同与竞争。

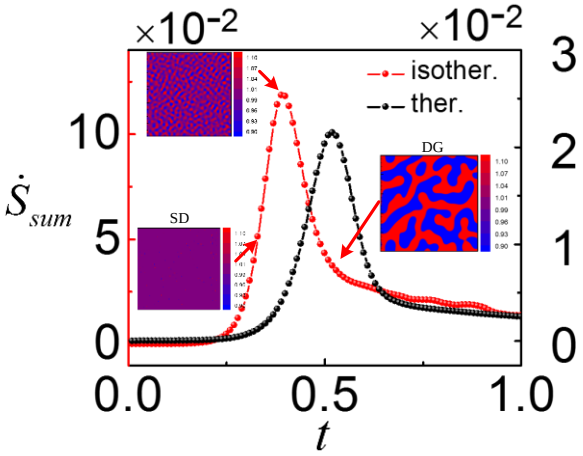

图 1 等温与非等温相分离过程熵产生速率演化特征的对比

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N21

专题代号:N

An effective statistical model of two-layer ReLU neural networks

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Abstract:

An attempt of understanding deep learning is to discover implicit biases underlying the training process of DNNs, such as the Frequency Principle (F-Principle), i.e., DNNs often fit target functions from low to high frequencies. Inspired by the F-Principle, we propose an effective model of linear F-Principle (LFP) dynamics which accurately predicts the learning results of two-layer ReLU neural networks (NNs) of large widths. This LFP dynamics is rationalized by a linearized mean field residual dynamic of NNs. Our work makes a step towards a quantitative understanding of the learning and generalization of general DNNs.

N22

专题代号:N

An analytical velocity field of spiral tips in reaction-diffusion systems

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关键词： velocity field，spiral tips，reaction-diffusion systems

摘　　要：Spiral waves are ubiquitous in diverse physical, chemical, and biological systems. The tip (or phase singularity) of a spiral wave is considered to represent its organizing center, and analytical formulas for its velocity contribute to the deep understanding of spiral wave dynamics. Here, we derive an analytical velocity field of spiral tips based on the variables of reaction-diffusion systems. From this velocity field, we can predict the velocities of spiral tips at time t as long as the values of the variables are given at that time. Numerical simulations with a two-variable reaction-diffusion equation are in quantitative agreement with the analytical results.

N23

专题代号:N

免疫生发中心里的动力学相变

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摘要：

面临各种病原的侵袭，健康生物体都能在较短的时间内生成抗体，恢复健康。淋巴结中的生发中心是完成这种抗体生成任务的主要外周免疫器官，通过 T 细胞和 B 细胞的相互作用，在很短的时间内能够完成抗原的识别，提取，加工和完整抗体的合成。动力学相变在这里发挥了独特的作用。

关键词: 统计物理，非线性科学，生物物理

N24

专题代号:N

FPUT 链稳定模式的失稳动力学

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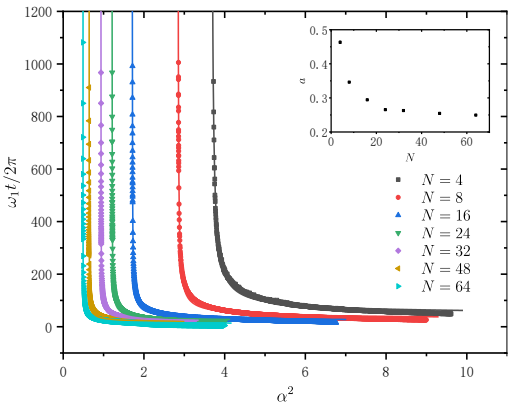
摘要：自 FPUT 问题于 1955 被提出以来，人们提出了许多理论来解释 FPUT 回归现象。1973 年，Bivins 发现了 FPUT-β 链存在某些特殊的正则模式，它们不与其他模式发生作用，称之为稳定模式。其中，又以波数 N/2 的模式最为稳定，N 是系统尺寸。通过数值模拟，Bivins 发现了稳定模式的失稳现象。由于 N/2 模式是最稳定模式，其失稳标志着系统进入全局混沌。因此研究 N/2 模式的失稳规律对于理解 FPUT 模型的非线性动力学具有重要意义。

我们研究了固定边界条件下 FPUT-α 与 FPUT-β 链中 N/2 模式的稳定性问题。在数值结果中，我们首次发现，N/2 模式的失稳时间与扰动强度的依赖关系很好地符合了 Nekhoroshev 拉伸指数律（图 1）。同时，利用 Floquet 定理与 Newton 公式，我们解析得到了扰动强度的失稳阈值与系统尺寸的依赖关系，与数值结果一致（图 2）。 我们的结果清楚地表明，系统相互作用势的对称性对体系的失稳过程有着极大的影响：对于非对称的 FPUT-α 模型，失稳阈值与 N 的关系为$\alpha^2\epsilon \approx 0.33/N - 0.86/N^2$；而对称的 FPUT-β 模型为$\beta\varepsilon \approx 4\pi/9N + 5\pi^2/4N^2$。我们的结果对于进一步理解小 N 条件下的能量均分问题提供了重要线索。



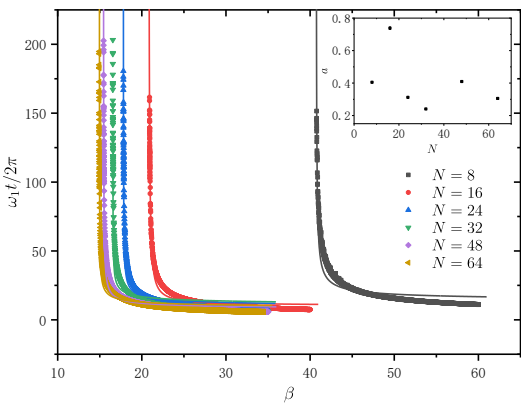


图 1 N/2 模式的失稳时间与扰动强度的关系(左为 FPUT-α 右为 FPUT-β)。两种模型的失稳时间与扰动强度的依赖关系符合 Nekhoroshev 拉伸指数律，FPUT-α 模型随着 N 的变大拉伸指数约为 0.25，而 FPUT-β 模型约为 0.3。

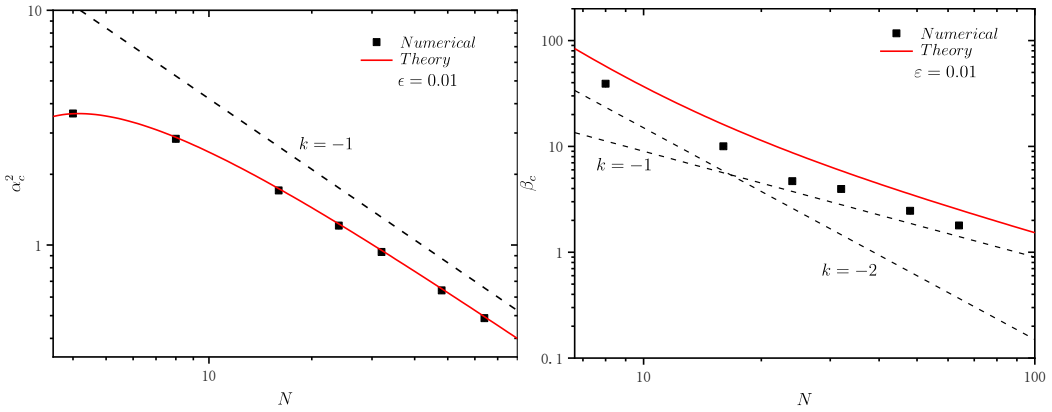


图 2 扰动强度 λ 与系统尺寸的依赖关系(左为 FPUT-α 右为 FPUT-β)。随着系统尺寸的变大，FPUT-α 模型的失稳阈值与系统尺寸的依赖满足幂律关系$\alpha^2 \sim N^{-1}$，而 FPUT-β 则是$\beta \sim N^{-2}$到$\beta \sim N^{-1}$的转变。

关键词：FPUT 问题 单模态解 稳定性

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N25

专题代号:N

Controllability and predictability of real temporal networks

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摘要：Links in most real networks often change over time. Such temporality of links encodes the ordering and causality of interactions between nodes and has profound effect on network dynamics and functions. Recent evidences recognize that link temporality of real networks is not completely random, yet it has been challenging to measure the regularity of temporal networks due to the entanglement of topological and temporal link patterns. Here we propose an entropy-rate based framework for quantifying the predictability of any temporal network. We validate our framework in various model networks, demonstrating that it indeed captures the intrinsic topological-temporal regularity while previous methods characterize only one aspect or only the regularity in link weight distributions. We apply the framework to a wide range of real networks and unveil the predictability profiles for different network categories. Interestingly, we find that a temporal network can be highly predictable even when both its topological and temporal regularities are very weak. Moreover, a recent discovery demonstrated that temporal networks are more controllable than their static counterparts in terms of control time, control energy and control path length. However, the underlying mechanism continues to elude us. Here we analytically and numerically investigate the controllability of temporal networks, finding that the (even tiny) change of link weights, not the order of snapshots, makes temporal networks more controllable. These findings deepen the understanding of temporality in complex systems.

The results in this talk are based on two studies in collaborations with Disheng Tang, Wenbo Du, Xianbin Cao and Xinya Zhang, Jie Sun.

N26

专题代号：N

多流行病传播动力学：多者异也

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摘要： The spread of infectious diseases, rumors, fashions, innovations are complex dynamical processes, embedded both in network and spatial contexts. While most of previous modeling work are based on single infection, the reality is that hundreds or even thousands of different infectious strains simultaneously spread around the world. In this talk, I will show that when two infections are allowed to circulate around in the population and the presence of potential interactions, the contagion dynamics could exhibit quite different behaviors, including the first-order outbreak transition, an avalanche scenario that much difficult to contain; In the spatial context, unexpected propagation modes are revealed such as receding waves or the standing wave; persistent spatial patterns are also possible, which make the eradication quite difficult. The uncovered dynamics are in sharp contrast with the case of single infection. These observations of "more is different" imply that the wisdom obtained from previous work based on single infection may not sufficient to capture the contagion complexities in the real world.

关键词：复杂传播 一级相变 渗流 斑图

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N27

专题代号:N

微观界面水的复杂行为及其生物效应

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界面水在许多材料和生物体系广泛存在，且受到界面结构、固液界面作用、自身氢键网络以及热扰动等因素影响，体现出非常复杂的行为。目前，人们对界面水分子如何参与界面物理和生物功能仍不够清楚。我将重点关注界面水的复杂的微观行为对界面性质的影响，以及生物如何利用这种微观行为调控生物功能，包括：(1)理论预言二维固体表面限域水氢键网络的集体有序行为导致常温下“不完全浸润的有序单层水”，解决了领域内一些争议问题，工作引发国内外一系列后续实验和理论工作； (2)与实验合作，提出抗冻蛋白控冰功能的关键分子机制：抗冻蛋白两个不同界面的残基结构及静电作用分别诱导了水的无序和有序行为，使得蛋白结冰面诱导有序水并诱导结冰，非结冰面诱导无序水并阻碍结冰；(3)理论揭示纳米受限三维空间和水分子参与导致双亲分子溶解状态在分散与聚集态之间发生自发转变。

关键词：界面水，氢键网络，生物功能，浸润，结冰

资助项目：国家自然科学基金（11290164,11674345,11204341），中科院青年科学促进会项目 2014233

N28

专题代号:N

二维胶体系统的动力学特性

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摘要：胶体是一个多尺度相互作用系统，由于存在着丰富的相和相变，一直是大家关注的热点。此外，胶体颗粒的尺寸介于几纳米到几微米之间，比原子分子的尺寸大很多，实验上容易对单个胶体粒子的位置和运动直接成像。因此，胶体为研究材料科学、物理化学和凝聚态物理中各种各样的问题，特别是为研究二维体系的动力学、相变和有序化等问题提供了理想模型。最近，活性胶体引起了广泛兴趣。研究活性胶体可以为揭示生物自组织的起源提供指导。本文综述了二维胶体系统的朗之万分子动力学特性，特别是脱钉特性。发现：纯排斥系统在脱钉点以上会发生从弹性晶体运动到弹性近晶运动，再到塑性流动的动力学转变，但不会出现类似于竞争排斥和吸引相互作用系统的团簇运动、甚至生命岛状运动等动力学有序结构；活性起源于一种弱的中短程吸引相互作用。

关键词：胶体 脱钉特性

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N29

专题代号:N

Simple mean-field theory for the Potts model

（Potts 模型的简单平均场理论）

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Potts model is one of the best known models for understanding continuous and discontinuous phase transitions. In this talk I will review a simple mean-field theory for the Potts model, which is exact on random graph ensembles. I will also discuss a surprising prediction of this theory, namely the existence of a discontinuous spontaneous color-symmetry breaking at certain fixed energy density. This discontinuous micro-canonical phase transition in random graphs is confirmed by micro-canonical Monte Carlo simulations, and it is also observed in bond-diluted finite-size lattice systems. [H.-J. Zhou, Phys. Rev. Lett. 122 (2019) 160601]

N30

专题代号:N

Applying multiple histogram reweighting method to study rare event on complex networks

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摘要：Large deviation theory and rare-event simulations have received growing attention in statistical physics, condensed matter physics, and interdisciplinary physics[1], such as fluctuation theorem, dynamical phase transition, etc. In this talk, I will present two concrete examples of large deviation in network science: atypical values of degree assortativity of configuration networks[2], and of the size of maximal connected component in percolation transition[3]. We first construct a Markov Chain Monte Carlo in canonical ensemble and then sample the degree assortativity and the size of maximal connected component across a wide range of inverse temperature. Finally, we apply a multiple histogram reweighting method[4] to obtain the probability distribution of degree assortativity and the size of maximal connected component. This method enables us to cover the rare-tails of the distributions in the allowable computational time. As by-products, we find that the fluctuation of degree assortativity shows an anomolously fast scaling with network size in highly heterogeneous networks and an explosive percolation transition against rare initial damage of nodes[5].

关键词： Large deviation; Rare event; Configuration model; Degree assortativity; Percolation

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N31

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Inflfluence of the degree of a complex network on heat conduction

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摘要：Devices made of nanotubes and nanowires networks are of great interest for applications and have caught increasing attention in recent years. In this work, we study heat conduction in a network model with nodes being atoms and links being one-dimensional chains of atoms. It is found that heat conduction in the complex network is fundamentally different from that of regular lattices. It depends very sensitively on the average degrees of complex networks and the degrees of nodes that are attached to the two heat baths. For example, when the two heat source nodes have the same degree *k*0, the heat flflux reaches a maximum at an optimized value of *k*0 and decreases with the increase of the average degree <k>. In other words, the source nodes with optimal degree k0 and the sparse network are more favorable to heat flflux. Thermal rectifification effect is found when the two heat source nodes have different degrees or the network model has multiple heat source nodes. Theoretical analysis is provided to explain the numerical results.

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N32

专题代号:N

能量特征在蛋白质结构评估及微小 RNA 预测问题中的应用

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本报告拟围绕蛋白质结构评估及微小 RNA 预测问题，阐述能量函数/能量特征在研究课题中的重要意义，进一步基于此介绍我们提出的 ANDIS（基于“原子对”距离和方位角统计信息的高性能势能函数）如何进行蛋白质结构评估，介绍我们提出的 plantMirP 进行植物微小 RNA 前体预测的算法。

N33

专题代号:N

链路预测理论：基于有向图和无向图的普适方法

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摘要：传统的链路预测方法一般只单一地针对于无向图或者有向图有效。本工作基于拉普拉斯变换，利用微扰理论，将无向图和有向图的链路预测统一起来，理论分析给出了的链路预测算法的精确解，进一步在数十种数据集上的实验效果显示，该方法不仅可以有效降低算法复杂度，而且预测效果也提高很多。该方法对于研究网络拓扑结构功能及其上的动力学有一定的启示意义。

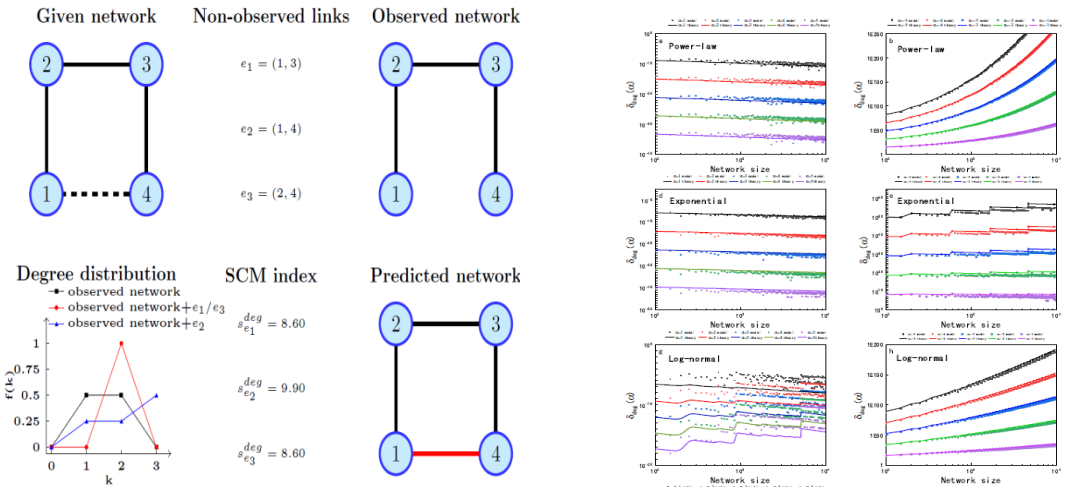

图 1 链路预测示意图(左) ；不同网络拓扑结构预测的理论和实验值（右）

关键词：复杂网络　链路预测 有向图 无向图

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N34

专题代号:N

Folding Cities

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摘要：Since the birth of the city, it has been an agglomeration of population and human interactions. Partially driven by optimizing the interacting efficiency, it has the tendency to grow in the third dimension – up to the sky, and in wake of the booming of modern building technologies, such gene is not dampened anymore, it even becomes the most distinguishable character of the city. This third dimension gives the city more possibilities and more interacting space, the city is actually folding more space to a small ground area where such agglomeration in the third dimension has been the more common case. And such folding behavior has profound impacts on the organizing and efficiency of the city. There have been tremendous evidences showing the sub-linear scaling relation between population and urban built-up area, yet this third dimension profile (total space volume of the city) has been rarely studied due to data limitation.

By investigating more than 60 cities in China, we show that there's a clear sub-linear scaling relation between the volume and population which indicates that even in three dimensions, the agglomeration effect is still the case (see Fig. 1). And we also show that within individual cities, the volume density profile follows a similar spatial scaling law discovered in the city [1]. From the city center to suburbs, the volume density decays in a power law way in most cities. Based on such volume density profile and clustering algorithm, we can identify different types of cities: fully developed, in need of renewal, new town mode. As taller buildings have higher volume, together with transportation networks, they dramatically change the space of cities which are no longer a 2-D space. By querying Amap API, we show the travel time from each building to the city center is not continuous with respect to the

distance to the city center by different means of transportation (bus + metro, car). And we show that most of these cities are car-favored where larger volume can be reached in shorter time by car. This indicates that our modern transportation network actually folds more space to central area.

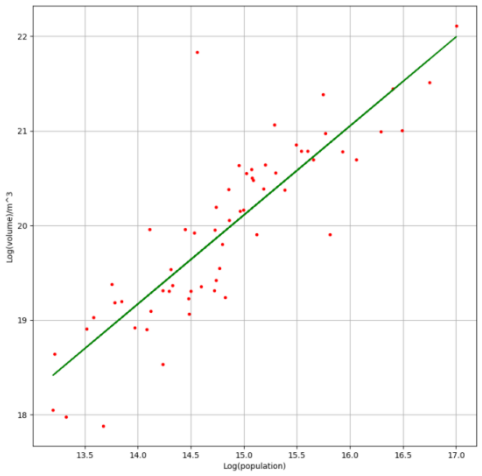

Figure 1: The sub-linear scaling relation between space volume and population for 60+ cities in China ($V \propto P^{0.94}$).

关键词：城市建模 标度律 空间形变

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N35

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Phase transition to synchronization in generalized Kuramoto model with low-pass filter

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摘要：A second-order continuous synchronization has been well documented for the classic Kuramoto model. In this work, we generalize the classic Kuramoto model by incorporating a low-pass filter (LPF) in the coupling, which serves as a simple but novel form of indirect coupling through a common external dynamic environment. The couping with LPF provides a bridge linking the direct coupling to the indirect one. Which serves as a minimal form of indirect interaction through a common external environment. We uncover that a first-order explosive synchronization turns out to be a very generic phenomenon in this generalized Kuramoto model with LPF. We establish theoretical results by providing a rigorous analytical treatment, which is validated by conducting extensive numerical simulations. The generalized Kuramoto model with LPF is the simplest exactly solvable case for indirectly coupled dynamical networks through a common external medium, which undergoes two distinct kinds of phase transitions towards synchronization depending on the cut-off frequency of the filter. Our study provides a new root for the emergence of first-order explosive synchronization, which could substantially deepen the understanding of the underlying mechanism of a first-order phase transition towards synchronization in coupled dynamical networks.

关键词： Phase transition, Kuramoto model, low-pass filter

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N36

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Burke-Shaw 系统的周期轨道研究

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摘要：混沌系统的奇怪吸引子是由无数条不稳定的周期轨道稠密覆盖构成的，周期轨道是非线性动力系统中除不动点之外最简单的不变集，它不仅能够体现出混沌运动的所有特征，而且和系统振荡的产生与变化密切相关。此外，在一个具有混沌性质的动力系统中，态空间的轨道通常是非常复杂的。两个相差无几的初值所产生的轨道，将会随着时间的推移按照指数方式分离，这种对初值的敏感性使得想要跟踪单个轨道比较困难，我们能做的是描述这个系统的一些平均的性质。周期轨道理论利用轨道展开，通过短周期轨道的系统计算即可给出精度较好的动力学平均，因此分析复杂系统的动力学行为时获取周期轨道具有十分重要的意义。

本文系统地研究了 Burke-Shaw 系统一定拓扑长度以内的周期轨道，提出一种基于轨道的拓扑结构建立一维符号动力学的新方法，通过变分法数值计算轨道显得很稳定。寻找轨道初始化时，两条轨道片段能够被用作基本的组成单元，基于整条轨道的结构进行拓扑分类的方式显得很有效。此外，讨论了周期轨道随着参数变化时的形变情况，为研究轨道的周期演化规律提供了新途径。本研究可为在其他类似的混沌体系中找到并且系统分类周期轨道提供一种可借鉴的方法。

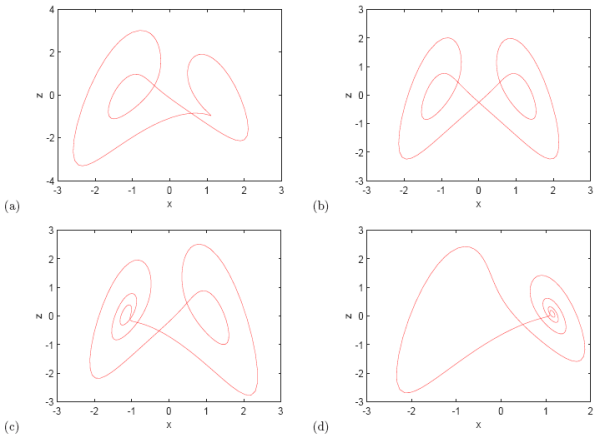

图 1 Burke-Shaw 系统不同拓扑长度的 4 条短周期轨道

关键词：Burke-Shaw 系统 周期轨道 变分法 符号动力学
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N37

专题代号:N

粗糙型固液界面的本征统计分析研究

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摘要：在匀质固液形核和晶体生长研究领域领域中，固液界面微观结构的演化和其中粒子的复杂集体转变机制是核心研究问题之一。由于实验的直接观测极具挑战，很多简单金属材料中固液转变的界面相变过程，如熔化相变【1】、准二维金属体系的固相-六角相和六角相-液相相变【2】、固液界面的粗糙化相变【3】等，粒子结构转变的微观机理仍多不清楚。Hernάndez-Guzmάn 和 Weeks 在 2009 年以胶体粒子构建模型固液两相平衡体系，在除去界面热毛细波动的影响的条件下以本征视角视察固、液相转变，获得了下本征固液界面过渡尺度远小于通常认为的界面厚度等新颖认识【4】。本次报告中，我们运用分子动力学模拟的方法构建了单质面心立方 Ni 和体心立方 Fe 在常压、熔点温度下的精确的固-液两相平衡态体系。统计分析固-液界面局域原子结构有序度以探究 Ni、Fe 体系固相至液相的结构转变的高时空分辨率视角下的微观动力学过程。我们还将展示我们对 Hernάndez-Guzmάn 和 Weeks 统计分析方法进行的进一步拓展。我们使用不同的结构序参量和作为参照的理想晶格点阵来表征本征界面。证明了界面的毛细波动使界面粗糙化，但仍可以得到本征的界面以区分固、液。发现了界面处固、液原子的结构序参量的统计分析的巨大差异表现，以及晶体类型、晶体学方向以及结构序参量无关。最后将讨论应用我们发展的本征统计分析方法所获得的固-液转变界面的本征厚度及其各向异性。

关键词：固-液界面、毛细波涨落、本征分析、界面结构、分子动力学模拟

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N38

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Supercoiling Dynamics under Mechanical Operations

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Abstract： DNA supercoils are prevalent and play the key roles in many cellular processes. During transcription, for example, RNA Polymerases (RNAPs) generate the supercoils along DNA by imposing torques on it. The supercoiling regulates the transcription in turn. Supercoils can also alter the conformation of the genome. In supercoiling dynamics, the torsion transport along DNA and the plectonemes hopping allow the long-range communication and the remote control between distant regions in cells.

Supercoils can be generated for topologically constrained DNA and the braid of polymers. The behaviors of supercoils depend on the torsion and tension. Employing the Brownian dynamics simulation of the worm-like chain model and along with the statistical mechanics of the DNA supercoiling, we study the supercoiling dynamics under an external torque and following a force operation, respectively. The supercoiling present the dynamics in two timescales, the torsion transport over one micrometer within 0.1 microseconds and the plectonemes generated in about 10 microseconds. Based on the separation of timescales between torque transport on DNA and phase-transition dynamics, we derived the time-dependent dynamics following the mechanical operations. Under the constant torque, we obtained a linear relationship between the excess linking number density and the fraction of the plectonemic phase during its growth. Notably, we have found that the increase of the linking number density follows a square-root of the time. For supercoils with given linking number, under a force quench from the original tension to a small one, the length of the plectoneme grows in response to the quench. We derived that the length of the plectonemes increases with the cube root of time at the intermediate times. The BD simulations confirm all these power laws. Inspired by the analysis of the

supercoiling dynamics under the mechanical operations, we established a phenomenological model to simulate the supercoiling under mechanical controls. This model facilitates the simulations of transcription regulated by supercoils in the timescales of minutes, even hours.

Key words: DNA supercoiling torque power laws phenomenological model

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N39

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Dramatic enhancement of interfacial thermal transport by mass-graded and coupling-graded materials

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摘要：With the dimension of materials shrinking into nanoscale, there has been growing interest in Kapitza resistance which inhibits the overall thermal transport. In this work, using the non-equilibrium Green's function method, we systematically investigate the optimized interfacial couplers with various gradient materials for phonon transport across one-dimensional atomic hetero-junction model. Relative to the optimized homogenous couplers, the mass-graded or coupling-graded structures are found to be applicable to improve the interfacial thermal conductance of two lead materials with both mismatched impedance and mismatched cutoff frequencies. For the couplers with both geometric graded mass and geometric graded coupling, the interfacial thermal conductance can be maximum enhanced (nearly up to sixfold enhancement on interfacial thermal conductance compared to the optimized homogenous case). The underlying mechanism of phonon transport enhancement by the last coupler is investigated by the phonon transmission coefficient: on one hand, this kind of coupler is able to maximally suppress the destructive interference for transmitted phonon waves; on the other hand, the constructive interference for the transmitted phonon is also largely improved. Our findings may offer guidance for advanced thermal interface materials design.

关键词：Interfacial coupler, Gradient material, Interfacial thermal conductance, NEGF method

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固体电介质中空间电荷引起的塞贝克效应

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摘要：我们从理论上证明，在空间电荷存在的情况下，固体电介质的塞贝克系数可以超出线性响应区域的相应极限。在这项研究中，我们考虑 p 型和 n 型载流子的共存，并通过质量作用定律将这两种载流子的浓度相互关联。如果仅考虑欧姆电导率或均匀分布的空间电荷，塞贝克系数跟线性响应区域中昂萨格倒易关系所给出的是一样，其绝对值处于 0 与 k/q 之间（k 为玻尔兹曼常数、q 为电子电荷）。但在非线性响应区域，如果本征载流子的浓度可以忽略而空间电荷出现一个不均匀的分布，昂萨格倒易关系不再成立，而塞贝克系数的绝对值处于 k/q 与 2k/q 之间，突破了线性响应区域的限制。

关键词：热电、塞贝克效应、空间电荷、电介质、昂萨格倒易关系

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N-P01

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一种计算量子微正则系综约化密度矩阵的近似方法

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摘要：微正则系综是统计物理的基本系综之一，对一个孤立量子系统，如果采用能量期待值为常数的约束条件则给出量子微正则（Quantum Microcanonical，简称 QMC）系综[1]。本文研究了 QMC 系综的子系统，提出了一种计算子系统约化密度矩阵的近似方法：在有限温度 T 时约化密度矩阵的对角元，近似等于 T=0 和 T=∞时约化密度矩阵对角元的线性组合。该方法的数值检验在 8 个自旋一维 XXZ 模型上进行，将其中 3 个自旋作为子系统，其他的作为环境，分为两个部分，分别从 QMC 和正则统计分布出发，通过准确对角化来计算约化密度矩阵。然后计算 T=0 和 T=∞时的约化密度矩阵对角元，按照近似方法将其线性组合，与上面的严格计算比较。结果表明近似组合与满足 QMC 分布的系统非常接近，而与满足正则分布的系统相差较大。如果逐渐减小子系统与环境的相互作用，则上述差别并不消失，只在某一值附近有所减小，而同时，近似方法与 QMC 系综子系统的分布始终符合较好。综上，从这一近似为研究孤立量子系统的子系统提供了一种有效方法。

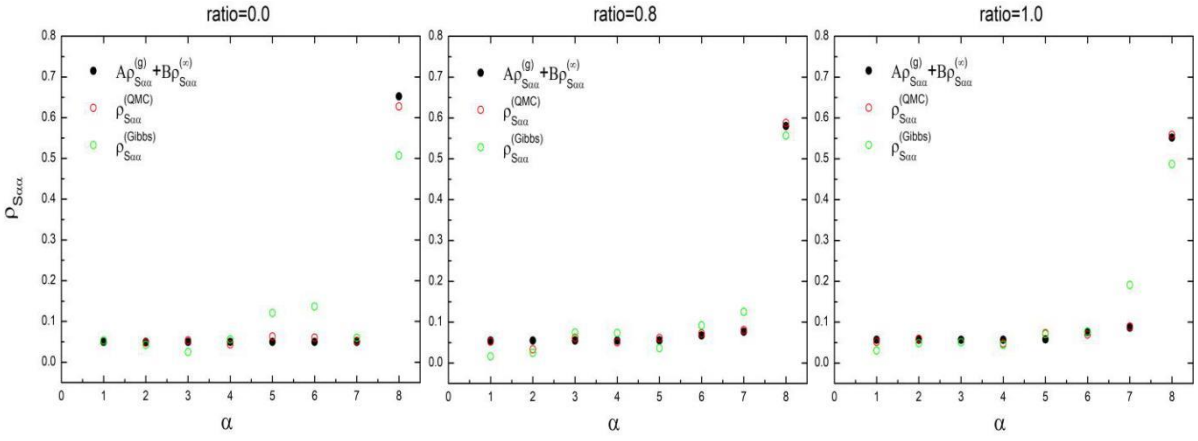

图 1 近似组合、QMC、Boltzmann-Gibbs 统计的约化密度矩阵对角元

关键词：XXZ，子系统，约化密度矩阵，量子微正则系综

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N-P02

专题代号:N

分会场专题名称：凝聚态理论与计算物理

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KSEA 相互作用对横场中若干 XY 模型基态性质的影响

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摘要：Dzyaloshinski 发现反对称的螺旋相互作用可以解释反铁磁性化合物中的弱铁磁性，后来 Moriya 给出了这个理论的微观基础。他们发现系统中还伴随有对称的螺旋相互作用但因其相对较小故而忽略了它。后来 Kaplan 发现单波段 Hubbard 模型中这种对称的螺旋相互作用不能忽略，随后 Shekhtman, Entin-Wohlman, 和 Aharony 三人发现这种不可忽略的对称螺旋相换作用可以解释 La_2CuO_4 的弱铁磁性，所以这种相互作用被称为 KSEA 相互作用。我们通过计算关联函数、von Neumann 熵和螺旋序参量研究了 KSEA 相互作用对横场中若干 XY 模型基态性质的影响。我们解析得出了每个模型的能量本征值和对应的本征失，并且利用数值方法计算了上述的物理量。通过分析这些物理量，给出了系统的相图。我们发现 KSEA 相互作用使 XY 模型的各向异性相变消失，并且当它足够大的时候，可以使 XY 模型外加 Dzyaloshinskii-Moriya (DM)相互作用或者三自旋相互作用时产生的零能隙相消失。

关键词：XY 模型，量子相变，KSEA 相互作用

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N-P03

专题代号:N

半导体激子极化激元系统中涡旋引起的非平衡相变

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摘要：涡旋属于二维系统的拓扑缺陷，在一定条件下顺时针和逆时针的涡旋会形成两两配对的束缚态，这称为 Berezinskii-Kosterlitz-Thouless（BKT）相变[1,2]。在本项研究研究中，我们考察了激子极化激元系统中的涡旋的动力学行为，以及由涡旋引起的 BKT 拓扑相变的性质。激子极化激元是半导体量子阱中的激子和微腔光子耦合后产生的一种半光半杂化态的准粒子，它构成了一种典型的带有外部驱动和内部耗散的非平衡量子流体，是一个很好的研究非平衡涡旋的平台。我们的理论研究基于 Gross-Pitaevskii 方程，同时考虑了外部驱动和内部耗散对系统的影响。我们用随机模拟方法对涡旋态的性质进行了研究，结果表明，涡旋在非平衡条件下也可以稳定存在，并且通过改变驱动泵浦 P_0 的强度可以改变涡流的分布，进而实现涡旋的配对，从而引发 BKT 相变（参见图 1）[3]。本项工作阐明了开放环境对涡旋动力学性质和配对机制的影响，也揭示了非平衡凝聚发生的物理机理。

(a) (b) (c)

(d)

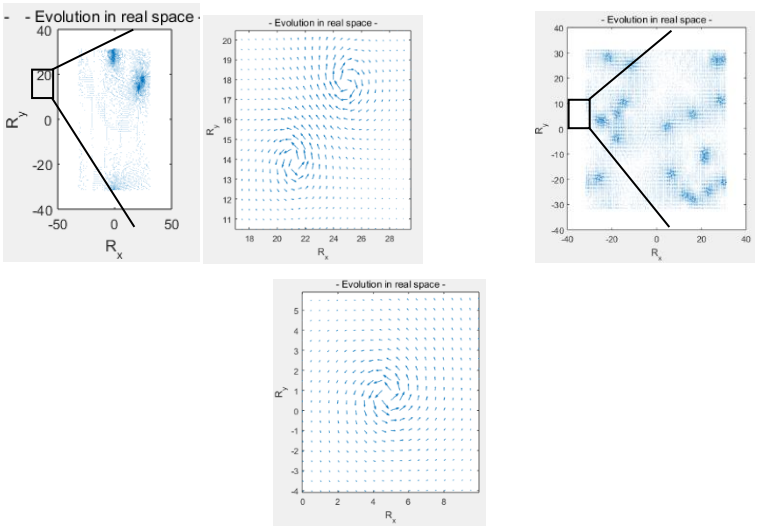

图 1.激子极化激元系统在不同泵浦强度 P_0 下涡流分布以及放大图：(a)和(b) P_0=2.0，(c)和(d) P_0=4.0。注意这里随着 P_0 改变，涡旋配对情况发生了变化。

关键词：激子极化激元，涡旋，G-P 方程，拓扑相变

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N-P04

N-P05

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复杂网络动态失效恢复中的相变动力学

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摘要：在现实世界中，当网络中的节点受到攻击时，网络的功能或结构将会受到一定的影响，甚至可能发生级联失效现象。但是对于一些系统，比如金融市场的突然崩盘，交通堵塞等，在经过一段时间的不活跃之后，这些受损的网络很大一部分会通过内部作用和外部作用重新活跃起来，这个过程会经常重复的发生，所以复杂网络的动态失效和恢复是一个重要的研究课题。我们建立了一个模型来模拟网络的失效和恢复过程，包括内部失效，外部失效，内部恢复和外部恢复。在三种不同的网络中（随机规则网络，ER 随机网络，无标度网络），通过模拟失效和恢复的过程，发现外部恢复将引起一级相变，内部恢复将引起二级相变，同时考虑两种恢复机制时，将出现回滞区域。此外，在相变点附近，我们发现三种不同的网络表现出不同的动力学特征，随机规则网络在相变点附近伴随一个成核的过程，网路中首先出现稳定的失效核，然后逐渐扩大到整个网络。ER 随机网络和无标度网络在相变点附近没有伴随成核的过程，在相变的过程中由高活性态会迅速变为完全失效态。最后，我们还研究相互依赖网络的鲁棒性。

关键词：复杂网络 自动失效和恢复 动力学性质

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N-P06

专题代号:N

非对称性对一维耦合转子晶格热输运行为的影响研究

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摘要：在低维系统中，傅里叶定律并不总是恒成立的，因此低维系统中的热输运问题吸引了很多关注。近年来，随着纳米技术的迅速发展，已经能够通过实验测量许多一维和二维微观材料的导热系数随尺寸的变化关系，证实了低维系统中的传热定律【1】。通常来说，一维动量守恒非线性晶格的能量扩散表现为反常的超扩散，但具有对称周期相互作用势的耦合转子晶格具有正常的能量扩散，相应正常的导热性质。对于具有动量守恒的非周期一维晶格，有观点认为，在一维动量守恒系统中非对称势能诱导正常导热，加入适度的非对称，可以使热输运从异常输运转变到正常输运【2】。但后续研究表明，这依然是一个有争议的结果，所观察到的正常热导行为可能是有限尺寸效应【3】。而非对称对具有像一维耦合转子这种周期势的晶格的影响还研究较少，有研究表明周期性可能是一位动量守恒晶格正常热输运的关键因素【4】。因此，本文定量的研究了非对称性对周期势的一维耦合转子晶格能量动量输运行为、流关联函数以及热导率的影响。为此，我们提出了一类具有动量守恒但相互作用势的非对称度不同的一维耦合转子晶格作为研究对象，采用了平衡分子动力学模拟的方法，我们知道，一维耦合转子晶格的能量扩散随着时间的增加时总是趋于正常扩散的【5】。在趋于正常扩散的这个阶段，我们发现，非对称性的加入，可以使一维耦合转子晶格转变到正常扩散的时间大大缩短，同时发现，非对称性越强，声模扩散速度越快，热模衰减速度也很快，很短时间内便能达到正常衰减规律，非对称性对流关联函数的影响也较为显著。都达到正常扩散后，相同温度下，非对称性越大，能量扩散系数反而越小，不对称程度对流关联函数衰减的影响变弱，不对称程度越大，热导率越小。

关键词：热导率 异常热输运 非对称

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N-P07

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Dramatic enhancement of interfacial thermal transport by mass-graded and coupling-graded materials

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摘要：With the dimension of materials shrinking into nanoscale, there has been growing interest in Kapitza resistance which inhibits the overall thermal transport. In this work, using the non-equilibrium Green's function method, we systematically investigate the optimized interfacial couplers with various gradient materials for phonon transport across one-dimensional atomic hetero-junction model. Relative to the optimized homogenous couplers, the mass-graded or coupling-graded structures are found to be applicable to improve the interfacial thermal conductance of two lead materials with both mismatched impedance and mismatched cutoff frequencies. For the couplers with both geometric graded mass and geometric graded coupling, the interfacial thermal conductance can be maximum enhanced (nearly up to sixfold enhancement on interfacial thermal conductance compared to the optimized homogenous case). The underlying mechanism of phonon transport enhancement by the last coupler is investigated by the phonon transmission coefficient: on one hand, this kind of coupler is able to maximally suppress the destructive interference for transmitted phonon waves; on the other hand, the constructive interference for the transmitted phonon is also largely improved. Our findings may offer guidance for advanced thermal interface materials design.

关键词：Interfacial coupler, Gradient material, Interfacial thermal conductance, NEGF method

基金项目：国家自然科学基金项目（NO.11890703）

N-P08

专题代号:N

逾渗模型中最大集团和骨干集团以及它们内部最大孔洞的大小分布

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摘要：在逾渗模型中，随着连接概率的增加，集团变大，到达临界点处时最大集团以一定的概率横贯整个空间。在二维空间，临界点处最大集团里的孔洞的大小分布指数与最大集团的分形维度之间满足一个超标度关系，并且孔洞的维度等于空间的维度 [1]。最近，侯等人研究了 Ising 模型在几何集团表象下的最大集团的分布，发现了双峰行为 [2]。为了更加深入地认识逾渗模型中的最大集团及其内部的孔洞， 我们采用蒙特卡罗方法仔细地研究了周期性边界条件下二维正方形格子上的键逾渗模型中的最大集团，最大骨干集团，及它们内部的最大孔洞的大小分布 [3]。我们发现这些分布的曲线除了具有一个明显的峰外，还具有小的凸起的部分（肩），特别地，最大集团里最大孔洞的分布展现出了良好的对称性。为了观察这些分布的性质， 我们在阈值附近改变连接概率的大小来观察峰与肩的变化，在上（或下）临界区观察到了双峰或类似高原形状的对称分布。在临界点附近，我们计算了的这些分布的方差，偏度和峰度等累积量，可以从这些累积量确定临界点和准临界点（pseudocritical point）。除此之外，对这些最大集团或孔洞是否发生缠绕进行分类， 我们发现它们出现的峰或肩的位置与它们发生缠绕的情况有显著的关系。

关键词：逾渗模型，集团大小分布，双峰行为

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Layzer 模型下压缩对 Rayleigh-Taylor 和 Richtmyer-Meshkov 不稳定性的影响

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摘要： 在改进的 Layzer 模型下，研究了压缩对 Rayleigh-Taylor (RT) 和 Richtmyer-Meshkov (RM)不稳定性的影响。从绝热方程$\frac{p}{\rho^{\gamma}}=const$可以看到，绝热系数 γ 可以作为一个表示不易压缩性的参量。为了能反映实际的不稳定性发展过程中界面处的压强、界面两侧密度的随界面运动速度的动态变化，我们还引入一个动态变化的驻点压强$P=p\pm\frac{1}{2}\rho U^2$，它可以将流体的实际密度与界面速度联系起来。借此，在 Layzer 模型的框架下，可以推导出关于可压缩流体的 RT 及 RM 不稳定性随时间发展的方程组，从而可以人为给静压强 p、界面两侧的静密度 ρ_{u0} 和 ρ_{l0}、界面两侧的绝热系数 γ_u 和 γ_l 赋值，这样就可以定量研究界面的振幅、速度和曲率半径随时间的演化。研究发现，对于 RT 不稳定性，界面上侧的绝热系数 γ_u 和密度有使 bubble 的振幅和速率增大，以及使早期阶段的曲率半径减小的效应；界面下侧的绝热系数 γ_l 和密度则有使振幅和速率降低，以及使早期的曲率半径增大的效应。然而，可压缩性并不影响 RT 不稳定性末态（bubble 速率不再随时间变化）的曲率半径。此外，当存在压缩性，我们发现可能会有上侧静态密度大于下侧却不能发生持续的 RT 不稳定性，或者上侧静态密度小于下侧但仍可发生持续的 RT 不稳定性的密度取值区间，这与不考虑压缩性的情况有明显的不同。对于 RM 不稳定性，上侧的绝热系数 γ_u 和密度有使振幅以及速率减小，以及使早期的曲率半径增大的效应。而下侧的绝热系数 γ_l 和密度则有使振幅及速率增大，以及使早期的曲率半径减小的效应。然而，对于 RM 不稳定性，当时间稍微增大时，可压缩情况下的曲率半径趋于与不可压缩的情况相同。

关键词：Rayleigh-Taylor 不稳定性　Richtmyer-Meshkov 不稳定性　Layzer 模型　压缩性

N-P10

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Giant Optimal Radiative Heat Transfer Driven by High Order Topological Insulators

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Abstract: We investigate the near-field heat transfer (NFHT) between high order topological insulators (HOTIs), which are protected by chiral symmetry and C_6 symmetry in present paper. It has been found recently that the localized zero-energy electronic edge states could change the NFHT behaviors substantially, when focusing on Coulomb interactions at a distance of nanometers. Here we find that high order topological protected states could also introduce novelty behaviors, such as the great enhancement of heat current compared to blackbody limit, the nonmonotonic vacuum-gap dependence of heat transfer and the stable maximal heat current. This may be used as a basis of topological devices' designing, to ensure a stable enhancement of heat transfer.

We use the nonequilibrium Green's function (NEGF) formalism within the random phase approximation (RPA).

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N-P11

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Quantum Entanglement Dynamics and Phase Transition of Spin-1 XXZ Model

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Abstract：

The critical properties and scale behavior of the antiferromagnetic spin-1 Heisenberg chain are analyzed by the method of renormalization group. According to the nature of the renormalization group, we divide the lattice points of the spin chain, and the three lattice points are a single block. Each block spin renormalizes into a new effective spin chain, the renormalization coupling coefficient can be obtained. The ground state negativity and entanglement entropy are calculated in the static quantum renormalization group scheme and the renormalization of negativity and entanglement entropy are obtained. To facilitate the study of the problem, we first select a fixed value of one parameter (the anisotropy parameter) and study the variation of entanglement with another parameter (crystal field parameter). Then we change the fixed value and study its variation. The phase boundary between the antiferromagnetic Neel phase, the Haldane phase and the large D phase is obtained. The first derivative of entanglement is studied with the parameter variation and the scale behavior exhibited near the phase transition point is calculated. It is found that the calculation results are consistent under different measurement methods.

In the low-energy dynamics of the system near the quantum critical point, different initial states are selected. This paper studies the evolution of two spin entanglement. The nature of entanglement at different times has been studied. It is proved that the scale behavior near the phase transition point is the same as one of the system under static. Related research helps to understand the nature of dynamic quantum phase transitions in non-equilibrium situations.

Keywords：
Renormalization group; Phase transition; Entanglement metric; Scale behavior; Dynamics.

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