2020 - 2021 年度报告 ANNUAL REPORT

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本册所列所有信息为2020年8月1日至2021年7月31日学术年期间

北京计算科学研究中心（以下简称中心）是隶属于中国工程物理研究院的独立法人单位，是以计算科学为牵引的多学科基础研究机构。中心成立于2009年8月。中心的定位是开展计算科学研究，促进科技发展，打造一个国际一流的开展计算科学及相关学科交叉研究的综合平台。

中心积极引进高层次人才，努力开展计算科学相关学科的交叉和创新研究，共有七个研究部：物理系统模拟研究部、量子物理与量子信息研究部、材料与能源研究部、复杂系统研究部、应用与计算数学研究部、力学研究部、计算方法研究部。截至2021年8月，中心的科研人才队伍包括16位讲座教授、3位教授、8位研究员、9位特聘研究员、6位特聘副研究员和2位工程师。另外，中心还有签约客座教授38位、博士后99位、博士/硕士研究生115位。他们的研究领域涵盖了数学、力学、物理学、化学、材料科学、计算机科学等多个基础、前沿领域。

2020-2021学术年期间，中心公开发表国际学术论文371篇，主办合办国内外学术会议9场，开设培训班5场，举办科技前沿讲座4期，邀请学术报告98期，接待来自10多个国家和地区的访问学者300余人次。中心还积极与国内外知名科研机构以合办会议、合带博士后、人员互访等丰富形式开展合作，努力推动学科交叉、加强学术交流。

作为一个基础性、跨学科、开放式的综合研究平台，中心将成为中物院在各个研究领域开展创新研究的重要支撑，开展对外科学技术交流合作的桥梁和纽带，高层次人才引进与培养的摇篮，同时填补我国计算科学相关学科交叉研究领域的空白。

中心定位与目标

1. 开展科学前沿研究

◇ 以计算科学研究为手段，以重大科学技术工程的实施和发展需求为牵引，积极引进海内外高层次人才，促进人才培养，开展基础性、前沿性、关键性和交叉性的研究工作；

◇ 加强对外学术技术交流，促进与国际知名科研机构的合作，搭建开放式、综合性、国际化的科研平台；

◇ 探索适于科研创新的管理体系，落实机制改革创新，提升我国科技自主创新能力，增强我国科技综合实力。

2. 发挥科学支撑效能

◇ 将科学前沿研究获取的新知识、新思想、新概念、新方法新手段通过多种方式转移到中物院其他研究机构；

◇ 与中物院其他机构合作，开展国家安全领域所需的新技术、新方法、新思路、新手段，乃至产生新工艺、新机理、新材料、新体系的研究；

◇ 拓展育新，根据中物院战略发展需求，布局和开展探索性、先导性研究，服务于院和国家未来发展的需要。

ABOUT CSRC

Beijing Computational Science Research Center (CSRC) is a multidisciplinary research organization under the auspices of the China Academy of Engineering Physics (CAEP). Established in August 2009, CSRC positions itself as a center of excellence in computational science research addressing current and critical issues in multidisciplinary of Mathematics, Mechanics, Physics, Chemistry, Materials Science, and Computational Science.

Mission of CSRC

◎ Carry out fundamental, frontier, critical, and multidisciplinary research with advanced computational approaches, thereby attract talents worldwide and train highly qualified research personnel, to support grand scientific development and technology innovation in China;

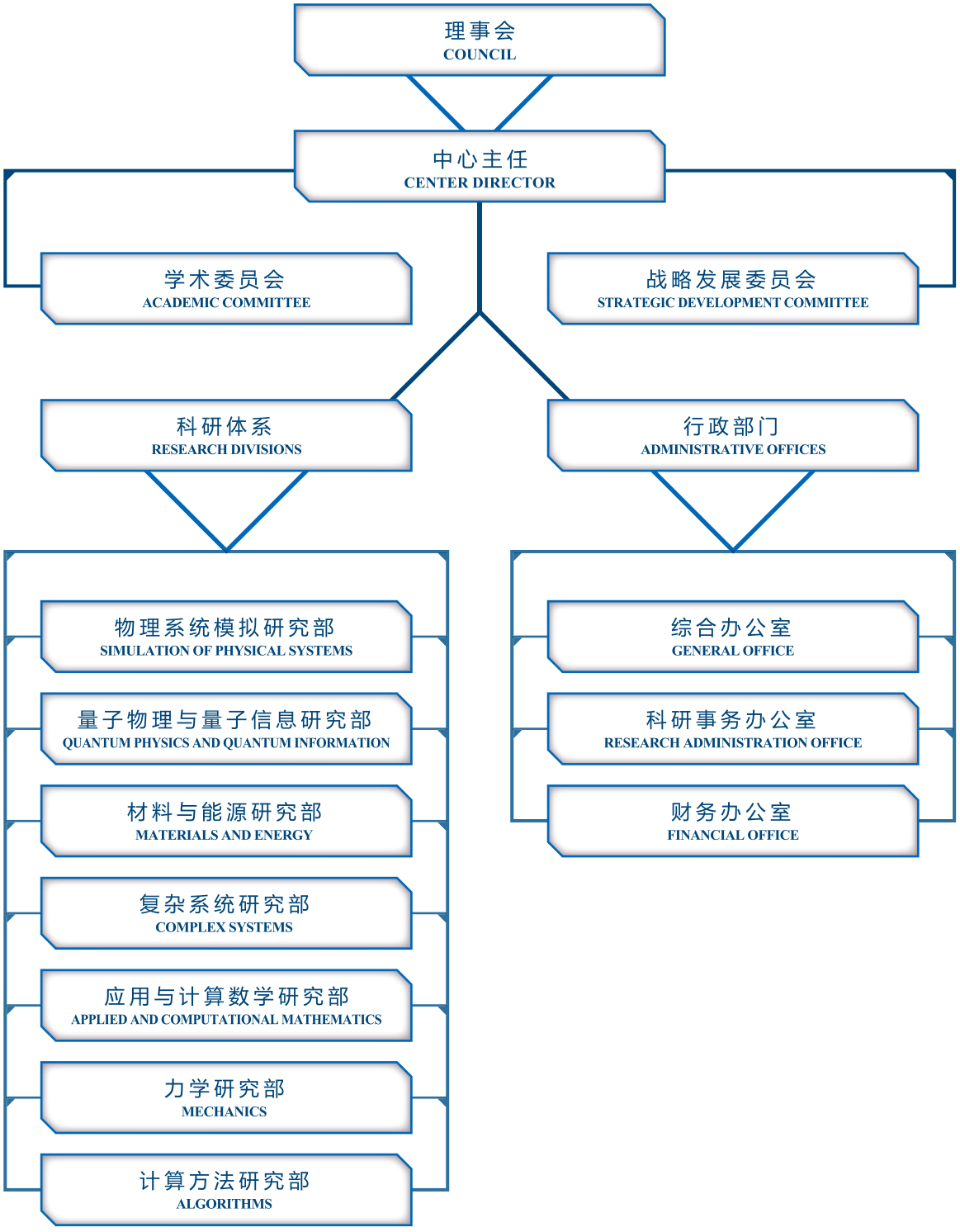
◎ Develop and maintain collaboration with research institutes elsewhere by building a comprehensive and internationalized research platform, to support academic and technological exchange and advancement;

◎ Innovate and reform organizational structures, management policies and methods for enabling creative and effective scientific research, to raise our national competence in technology innovation and enhance our comprehensive strength in science and technology.

Specifically, CSRC supports the development and implementation of grand challenging projects in natural science and engineering where computational modeling and simulation play a key role. CSRC also encourages its members to engage in the development of computational algorithms and software.

As of August 2021, CSRC has 42 faculty members, 2 engineers, 38 associate members, 99 postdoctoral fellows and 115 students. With its talented research staff, CSRC has established the following seven divisions: Simulation of Physical Systems, Quantum Physics and Quantum Information, Materials and Energy, Complex Systems, Applied and Computational Mathematics, Mechanics, and Algorithms. In research performance, CSRC has published 371 papers, organized 9 academic conferences and workshops, 5 tutorials, 4 colloquium on scientific frontiers, and 98 CSRC seminars. CSRC has also forged partnerships with many prestigious universities and research institutes around the world.

ORGANIZATION 中心组织构架



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OBSERVATION OF ENERGY-RESOLVED MANY-BODY LOCALIZATION

(By Qiujiang Guo, Chen Cheng, Zheng-Hang Sun, Zixuan Song, Hekang Li, Zhen Wang, Wenhui Ren, Hang Dong, Dongning Zheng, Yu-Ran Zhang, **Rubem Mondaini**, Heng Fan, H. Wang)

The thermalization of an isolated quantum system, well understood in the framework proposed by the ETH ansatz, breaks down in the presence of sufficient disorder, resulting in the preservation of local information under the evolution at arbitrarily long times [1]. In a different perspective, this phenomenon can be interpreted as a generalization of the phenomenon of Anderson insulating behavior, which can occur for non-interacting disordered quantum systems [2]. In the many-body localization (MBL), there are two competing knobs that lead to delocalization (interactions) and localization in real space (disorder). Early experimental attempts have demonstrated that this interplay can be observed in the context of ultracold atoms trapped in (quasi-) disordered optical lattices [3]. More recently, theoretical investigation in CSRC have pointed out that the onset of localization systematically depends on the energy of the system, defining a many-body mobility edge. Nonetheless, challenges from analytical arguments describe that the existence of such phenomenon would destabilize the existence of a localized phase [4]. To settle this debate, Rubem Mondaini from the Beijing CSRC sought for a way to describe this phenomenon experimentally. By proposing and collaborating with Prof. Haohua Wang (Zhejiang University) and Prof. Fan Heng (IOP) he pushed the idea that existing platforms of interacting superconducting qubits are the ideal setting for understanding this physics, outpacing experiments in cold atoms.

The main idea is that in a quench problem, the initial state fully encodes the total energy of the system (within the regime the system is still isolated from perturbations from the environment) and, as such, would allow to probe when localization occurs with energy resolution. That is, by initializing a product (Fock) state $|\Psi_0\rangle$, the unitarily time-evolved wave function $|\Psi_t\rangle = e^{-\mathrm{i}HT}|\Psi_0\rangle$ preserves the total energy $\langle\Psi_t|H|\Psi_t\rangle = \langle\Psi_0|H|\Psi_0\rangle = E$, under the effective Hamiltonian of the superconducting quantum processor

$$\frac{H}{h} = \sum_{\{m,n\}\in N} J_{mn}\left(\sigma_m^+\sigma_n^- + \sigma_m^-\sigma_n^+\right) + \sum_m V_m\,\sigma_m^+\sigma_m^-, \quad (1)$$

where $\sigma_n^-\left(\sigma_m^+\right)$ is the lowering (raising) operator for qubit Q_m, and the first term runs at pairs of qubits Q_m and Q_n . The schematics of the device is given in Fig. 1.

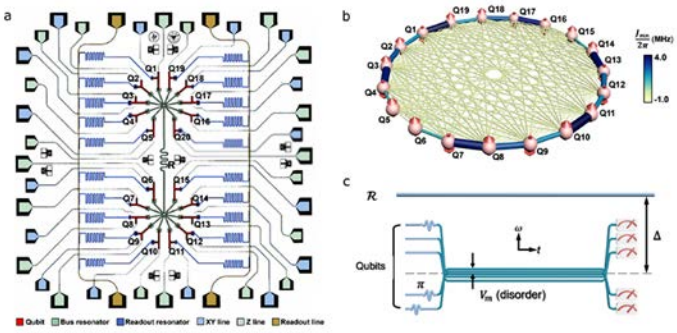

Fig. 1. Quantum processor and experimental pulse sequence.} a. False color image showing 20 superconducting qubits, b. Schematic representation of the effective all-to-all coupling strengths, $$, among the 19 qubits (spins); c. Experimental pulse sequence in the frequency vs. time domain for observing energy resolved MBL.

By carefully selecting initial states, one can understand how the onset of localization takes place at different energies. For that one can use a local observable that dynamically tracks the occupation

of particles (photons). If the occupancies are largely preserved for a specific initial state, one then says that memory of the initial conditions is observed, and many-body localization takes place. By compiling such analysis for a variety of initial states, we end up describing an experimental observation of a many-body mobility edge, with remarkable agreement with its numerical counterpart using experimentally calibrated parameters, see Fig. 2.

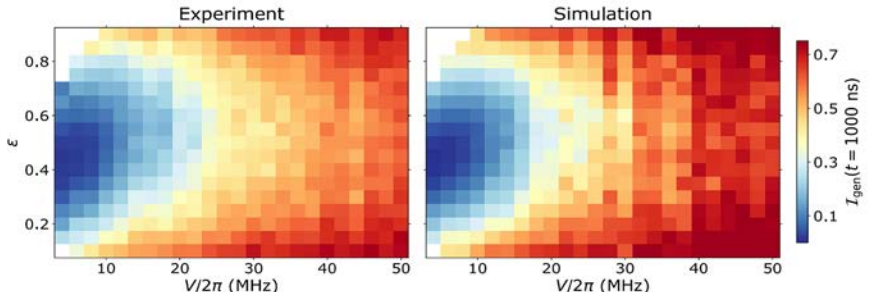

Fig. 2. MBL phase diagram—experiment versus simulation. Disorder-averaged imbalance measured at t = 1,000 ns (left) compared with the numerical simulation of the dynamics taking into account all device parameters except decoherence (right).

These results, published in Nature Physics [5], thus go beyond of previous experimental explorations of this transition which have often neglected the energy dependence on the onset of localization. The precise understanding of how the triggering of the MBL phase is influenced by this extra variable has direct consequences to potential technological applications on a quantum memory instrument. Further generalizations of this study aim in investigating the possibility that quenched disorder is not the only mechanism in which isolated quantum system may fail to thermalize. In particular, if a non-random linear potential is applied, one can realize the many-body version of the well-known phenomenon of Stark localization. One of the direct outcomes is that a quantum memory device using the MBL as a building block of memory preservation would then not need quenched disorder as a fundamental step, thus facilitating reproducibility. This is under investigation by the authors.

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[1] Rigol, M., Dunjko, V. & Olshanii, M. "Termalization and its mechanism for generic isolated quantum systems". Nature 452, 854–858 (2008)

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[5] Qiujiang Guo; Chen Cheng; Zheng-Hang Sun; Zixuan Song; Hekang Li; Zhen Wang; Wenhui Ren;, Hang Dong; Dongning Zheng; Yu-Ran Zhang; Rubem Mondaini*, Heng Fan*; and H. Wang* "Observation of energy-resolved many-body localization", Nature Physics 17, 234–239 (2021)

实验观测到能量分辨的多体局域化现象

(郭秋江，程晨，孙政杭，宋紫璇，李贺康，王震，任文慧，董航，郑东宁，张煜然，**Rubem Mondaini**，范桁，王浩华)

孤立量子系统的热化现象在本征态热化假设框架下已经被很好的理解，但当系统的无序足够大时，系统不但不会热化，反而在无穷长的演化时间下局域的信息仍有保留[1]。从另一个角度来看，这一现象可以看作是无相互作用无序系统中安德森局域化在相互作用多体系统中的推广[2]。在多体局域化(MBL)现象中，存在两个相互竞争的参量，一个是相互作用强度，会导致系统热化；另一个是无序强度，会导致系统在实空间局域化。早期的实验表明这种竞争机制可以通过囚禁于准无序的光晶格中的超冷原子系统观察到[3]。最近，来自北京计算科学研究中心的研究团队理论上指出多体局域化现象的出现依赖于系统的能量，这种能量的依赖定义了多体迁移率边界。然而，其他理论工作指出这种现象的出现将使局域化的存在变得不稳定，这为多体迁移率边界理论带来了挑战[4]。为了解决这场争论，来自北京计算科学研究中心的 Rubem Mondaini特聘研究员找到了一种实验上的方法来描述这一现象。通过与浙江大学王浩华教授和物理所范珩研究员合作，他提出现有的相互作用超导量子比特系统是理解多体局域化物理机制的理想平台。他们的想法是在一个弛豫过程中，初态完全决定了系统的总能量(环境对系统的微扰可以被忽略)，当系统演化时，可以从系统能量上分辨局域化是否发生。也就是说，给定一个初始的Fock态$|\Psi_0\rangle$，幺正演化波函数$|\Psi_t\rangle = e^{-iHT}|\Psi_0\rangle$ 使总能量$\langle\Psi_t|H|\Psi_t\rangle = \langle\Psi_0|H|\Psi_0\rangle = E$ 保持不变，其中 H 为超导量子处理器的有效哈密顿量，具体形式为:

$$\frac{H}{h} = \sum_{\{m,n\}\in N} J_{mn}\left(\sigma_m^+\sigma_n^- + \sigma_m^-\sigma_n^+\right) + \sum_m V_m\,\sigma_m^+\sigma_m^-, \quad (1)$$

这里 $\sigma_n^-\left(\sigma_m^+\right)$ 为量子比特 Q_m 的上升下降算符，上式第一项中 J_{mn} 代表不同的比特 Q_m 和 Q_n 之间的耦合。实验平台的结构见图1。

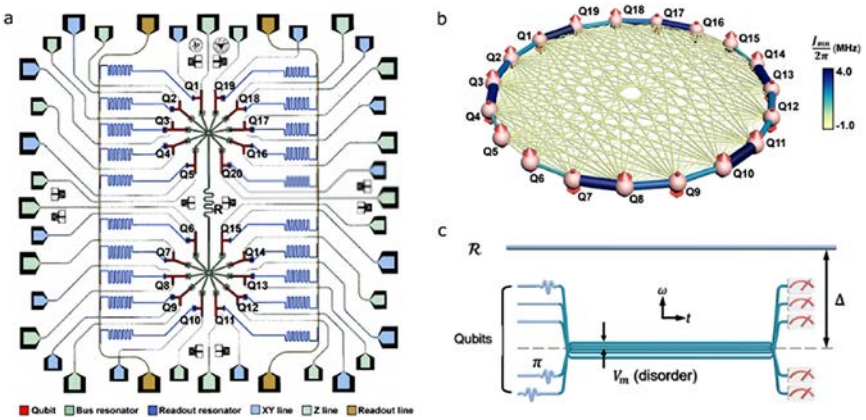

图 1　量子处理器结构和实验上的脉冲序列示意图。a. 20个超导量子比特处理器结构图 b. 19个量子比特（自旋）之间有效的全局耦合示意图。 c 能量分辨的多体局域化现象中频率-时间分布的实验脉冲序列。

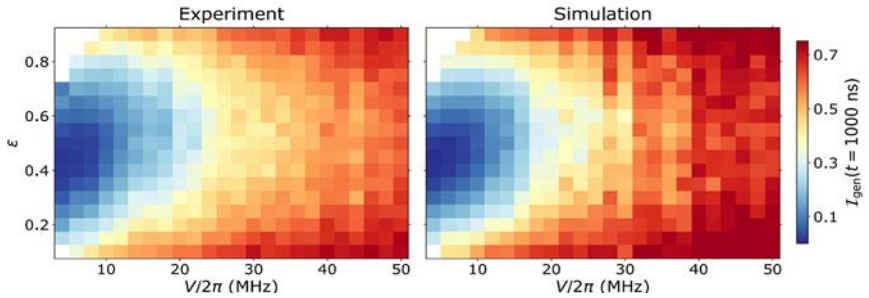

图 2　多体局域化相图-实验和数值结果。左边是在1000ns时测量得到的无序平均的不平衡度，右图是考虑了除退相干之外的所有的器件参数的动力学演化的数值结果。

通过仔细选择初始状态，就可以知道在不同的初始能量下多体局域化是如何发生的。为此，他们利用一个局域可观测量，来动态跟踪每个比特的占据数(光子数)。如果初始的占据数在演化时变化很小，就可以认为初始状态的信息被保留，也就是说多体局域化发生。通过对大量的初态做类似的分析，他们在实验上观察到了多体迁移率边界，与相同参数下的数值结果符合的很好，结果见图2。

相关结果发表在Nature Physics[5]上。这一结果超越了之前关于多体局域化转变的实验结果。之前的实验结果忽略了多体局域化现象出现的能量依赖。从应用角度而言，准确理解能量这一参量是如何影响多体局域化的发生对量子存储器的潜在技术应用有直接意义。在这些研究结果的基础上，他们进一步的想法是研究无序是否是孤立的量子系统无法热化的唯一机制。他们发现在给比特作用一个非随机线性势时，可以实现多体版本的Stark局域化现象。这一研究的潜在应用之一是在利用多体局域化作为存储模块构建原理的内存设备中，产生无序作用势不再作为基本步骤，这使存储器件变得可重复。目前相关研究正在进行中。

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[1] Rigol, M., Dunjko, V. & Olshanii, M. “Termalization and its mechanism for generic isolated quantum systems”. Nature 452, 854–858 (2008)

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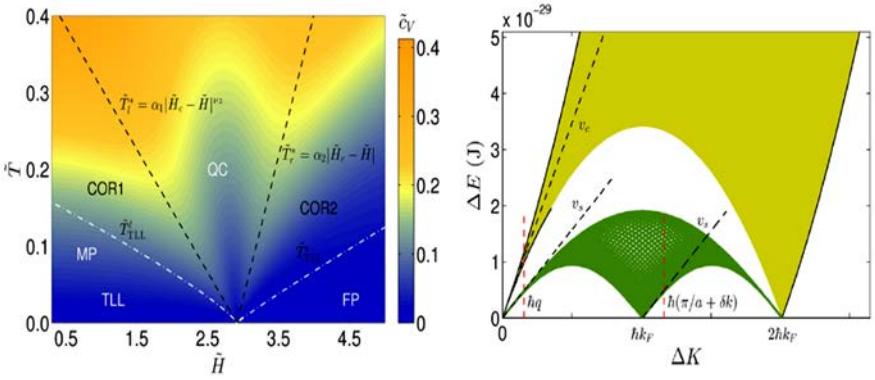
SPIN-CHARGE SEPARATION IN ONE-DIMENSIONAL REPULSIVE FERMI GASES

(By Feng He, Yu-Zhu Jiang, **Hai-Qing Lin**, Randall G. Hulet, Han Pu, and Xi-Wen Guan)

Interacting quantum many-body systems with rich internal degrees of freedom pose a formidable challenge for theoretical study. For decades, many efforts have been devoted to understand that how interactions between fermions affect the state of a quantum liquid at low temperatures, and thus a wealth of approximate formalism has been developed, such as Landau's Fermi liquid theory, Green's function approach, and Tomonaga-Luttinger liquid (TLL) theory etc. Of special importance to the one-dimensional system, the TLL usually refers to the collective motion of bosons that is significantly different from the free fermion in the Fermi liquid. One of hallmarks for 1D physics is the splitting of low-lying excitations of interacting fermions into two separate TLLs, i.e., the separated quasiparticles carry either spin or charge. This phenomenon is known as spin-charge separation. Although TLL physics can be directly obtained from the Bethe Ansatz (BA) solutions, its feature is easily disrupted once backward scattering is included or when the system is strongly disturbed by thermal fluctuations at quantum criticality.

In this work, Prof. Haiqing Lin from the Beijing CSRC collaborating with Prof. Xi-Wen Guan's group from Innovation Academy for precision Measurement Science and Technology (CAS) together with Prof. Randy Hulet and Prof. Han Pu from Rice University study the universal properties of spin-charge separated and disrupted liquids in a repulsive spin-1/2 Fermi gas. They present analytical results of thermodynamic and magnetic properties of the system which essentially mark the spin charge separated liquids below a lower critical temperature, the universal scaling behavior of free fermion quantum criticality above an upper critical temperature, and the disrupted quantum liquids in between. They also evaluate exact low-lying excitations that rigorously indicate the separation of the particle-hole continuum in the charge sector from the two-spinon spectrum in the spin sector. Such separated spectra are exploited to calculate the charge and spin dynamic structure factors (DSFs) and to probe the emergent phenomena such as spin-charge separation and fractional excitations in Fermi gases.



The Left Panel: Phase diagram determined by the contour plot of specific heat. MP, FP, and QC represent the mixed phase, fully polarized phase, and quantum critical region, respectively. The crossover region between TLL and QC are denoted as COR1 and COR2, which coincide with the incoherent Luttinger liquid.

The Right Panel: Exact low energy excitation spectra in charge (yellow green) and spin (dark green) sectors. The dark green shows the continuum of two-spinon excitation. The black dashed line in each sector represents the corresponding sound velocity for that type of excitation, which is an explicit proof of the spin-charge separation.

一维SU(2)费米气体中的自旋-电荷分离

(何丰，姜玉铸，**林海青**，Randall G. Hulet，浦晗，管习文)

粒子间复杂的相互作用和系统丰富的内部自由度通常给系统物理特性的描述带来巨大挑战。特别是对费米子之间的相互作用如何影响低温下量子液体状态的研究已经有50多年的历史，期间人们发展了大量的近似理论和唯象理论来描述和理解这种普适的低能物理，如朗道-费米液体理论成功的描述了高维电子体系、重费米子、近藤杂质等体系的低能量子流体特性。在一维量子多体物理中，朝永-拉亭戈液体理论以及量子多体的长程关联通常被用来描述一维多体系统的低能普适行为。一维相互作用费米子的低能激发通常会分裂成两支独立的朝永-拉亭戈液体，它们分别刻画携带自旋和电荷的准粒子，这种现象被称为自旋电荷分离，这也是一维量子体系所独有的多体物理现象。尽管这方面的研究也有40多年的历史，并在一些固体材料中观测到这种奇特现象的一些证据，包括德国马普所的Bloch实验组在Science 367, 186 (2020)发表的关于自旋-电荷分离的动力学研究，然而对于这种现象至今缺乏令人信服的实验验证。自旋电荷分离现象涉及两个重要的特征：1) 自旋-电荷分离的准粒子激发谱；2) 分离的自旋和电荷朝永-拉亭戈液体。事实上已有的几个固体物理实验基本上都是观测到前者的特征，或与分离激发谱相关的输运特性，这方面的研究一直是理论和实验研究难题。

另一方面，杨振宁和Gaudin教授分别在1967年求解了一维自旋-1/2 delta-函数相互作用的费米气体，即Yang-Gaudin模型，这个模型成为量子统计物理中的典范。然而，该模型精确解所给出的方程极其复杂，发现其中所蕴含的物理一直是数学物理中的挑战性难题，从而阻碍了该模型在实际实验中的应用。北京计算科学研究中心林海青教授与中科院精密测量科学与技术创新研究院管习文团队, 美国莱斯大学Randy Hulet和浦晗教授合作，通过量子可积系统理论，得到一维超冷费米气体独特的分数化准粒子和自旋-电荷分离现象的精确结果，并给出实验验证这些新奇的一维多体物理现象的具体方案，通过研究杨-Gaudin模型的精确解，首次精确计算了电荷自由度中的粒子-空穴集体激发谱和双自旋子(分数化准粒子)激发谱，进而得到零温和有限温度下自旋-电荷分离的普适关系及量子临界现象的普适标度，参见左图。他们发现一旦激发涉及反向散射或在临界区受到热涨落的强烈干扰，电荷-自旋分离的朝永-拉亭戈液体特性就会失效，在临界区将会涌现出非相干的拉亭戈液体区(COR区)，它表现出不同于临界区(QC)自由费米临界标度关系。在该文的最后部分，他们证明了一维超冷费米原子体系的动力学结构因子不但可以用来观测自旋电荷分离的激发谱，而且可以用来验证朝永-拉亭戈液体动力学关联函数，并据此提出了实验验证自旋-电荷分离现象的具体方案。他们的研究结果提供了对分数化准粒子、自旋电荷分离、量子临界性和非相干拉亭戈液体的精确理解，给出了量子多体物理的一个优美范例，并为将来可能的基于准粒子的量子精密测量提供了有意义的理论基础。

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[1] Feng He, Yu-Zhu Jiang, Hai-Qing Lin*, Randall G. Hulet, Han Pu, and Xi-Wen Guan*: Phys. Rev. Lett.125, 190401 (2020).

ASYMMETRIC LIGHT SCATTERING ON HETERODIMERS MADE OF AU NANORODS VERTICALLY STANDING ON AU NANODISKS

(By Yunhe Lai, Ximin Cui, Nannan Li, **Lei Shao**, **Wei Zhang**, Jianfang Wang, **Hai-Qing Lin**)

Directional light control at nanoscale shows great potential in applications such as holograms, optical neural networks, and ultracompact photonic circuits. Plasmonic nanostructures with designed geometrical shapes or complex architectures have been employed to manipulate light directionally. The interaction among the electric dipole and multipole resonances in plasmonic nanostructures enables the wavefront reshaping of light, leading to directional light scattering behaviors. However, traditional methods for directional light control suffer from complicated fabrication procedures and large footprints. In this work, heterodimers are constructed out of chemically grown Au nanodisks and Au nanorods, with the nanorod sitting vertically on the nanodisk, and their directional light scattering behaviors are studied. When the nanorod is located off the center of the nanodisk, the incident light is scattered asymmetrically by the heterodimer, producing a crescent-shaped far-field scattering pattern. The light scattering directionality of the heterodimers is further proved to be highly dependent on the aspect ratio of the nanorod, the relative position of the two nanocrystals, and the orientation of the nanorod. The study provides a solid and useful foundation for the directional light manipulation in ultracompact nanophotonic systems.

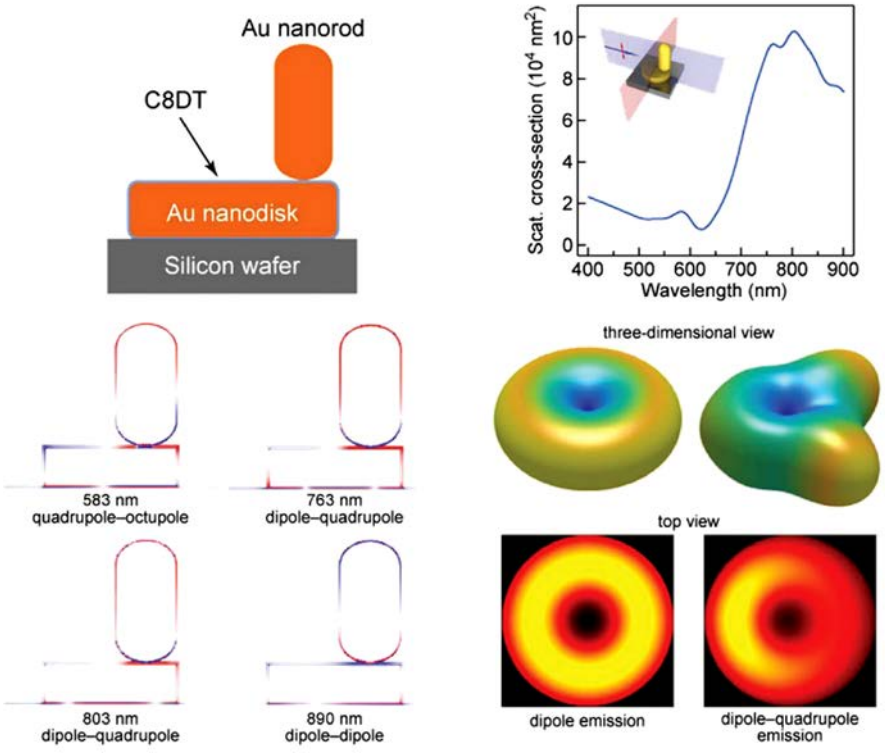

Fig. 1. FDTD simulation showing the resonance modes supported by the heterodimer with Au nanorod sitting vertically on Au nanodisk and their far-field emission patterns.

金纳米盘–纳米棒异二聚体纳米天线的非对称光散射性质研究

（来云鹤，崔熹旻，李楠楠，**邵磊**，张伟，王建方，**林海青**）

在纳米尺度上实现光的定向传播控制在全息成像、光学神经网络构建和高集成度光子电路等方面有着巨大的应用潜力。在已有的报道中，人们一般通过设计特定几何形状的等离激元纳米结构或者其复杂的复合结构来实现上述对光传播的定向控制。这些结构中的电偶极子和多极子共振模式之间的相互作用可以用于光的波前整形，从而导致定向光散射行为。然而，传统的方法一般需要复杂的样品制备工艺，也很难做到极小的结构尺寸。本工作利用由化学生长合成得到金纳米盘和金纳米棒构筑成的异二聚体来实现对入射光的定向散射。复合结构由分子组装工艺将纳米棒垂直放置在纳米盘上而形成，当纳米棒远离纳米盘的中心时，入射光被异二聚体不对称散射，产生新月形远场散射图案。进一步的研究表明异二聚体的光散射方向性高度依赖于纳米棒的纵横比、两个纳米晶的相对位置、以及纳米棒的取向。该研究为超高集成度纳米光子学系统中的定向光操纵提供了坚实的基础。

◀ 图 1　有限时域差分方法模拟计算得出的金纳米棒-纳米盘异二聚体结构中的光学共振模式及其远场辐射图案。

References:

[1] Y. H. Lai, X. M. Cui, N. N. Li, L. Shao, W. Zhang, J. F. Wang*, H.-Q. Lin*, “Asymmetric light scattering on heterodimers made of Au nanorods vertically standing on Au nanodisks”, Adv. Opt. Mater. 9: 2001595 (2021).

ELECTROPHORETIC PLASMONIC INK FOR DYNAMIC COLOR DISPLAY

(By Jiapeng Zheng, Tsz Him Chow, **Shasha Li**, Jianfang Wang, **Lei Shao**)

Plasmonic metal nanostructures generate vivid colors with high spatial resolution. Active control of plasmonic pixels by electrical means, which is compatible with integrated circuit technologies, is a promising technique for dynamic full color reflective display. However, the development of electrical plasmonic display is still limited by the difficulties in cost-effective construction of active plasmonic pixels over large areas. This study demonstrates the achievement of electrical plasmonic display in full color by electrophoretic movement control of plasmonic noble metal nanocrystals in an organic electrolyte solvent. The structures were designed by electrodynamic simulation and their movement dynamics was predicted by calculation. The plasmonic electrophoretic display was then realized in experiments. Such plasmonic display is of high contrast, high saturation, and can be switched reversibly for many cycles. This is by far the first implementation of electrophoretic color display based on colloidal plasmonic nanocrystals. This work will help remove obstacles for further commercialization of the electrical plasmonic display. The fabricated plasmonic 'ink' can be also applied in various all-nanocrystal electronic devices and color industry.

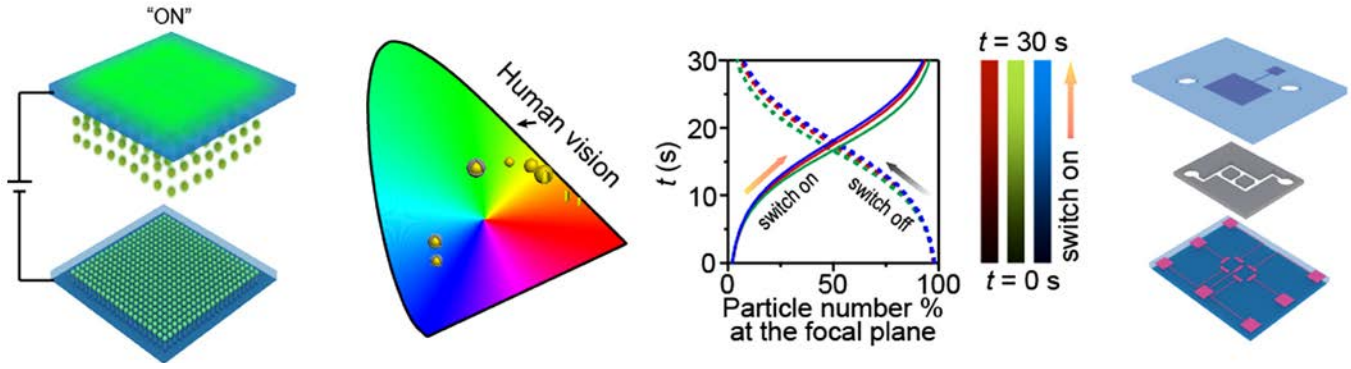

Fig. 1. Electrophoretic color display by actively controlling the movement of plasmonic metal nanocrystals.

用于电泳动态彩色显示的等离激元“电子墨水”

(郑嘉鹏，Tsz Him Chow，李莎莎，王建方，邵磊)

具有等离激元共振特性的金属纳米结构可以用于产生具有极高空间分辨率的鲜艳色彩。这种结构因而有希望用于实现全彩的反射式显示技术，促进当前市场上黑白电子书向彩色电子书的技术迭代。实现上述技术的关键在于通过电子学方法来控制单个等离激元彩色像素点，实现动态的颜色开关控制。然而，目前电控的动态等离激元器件的制备成本仍然居高不下。本研究利用等离激元贵金属纳米晶颗粒在有机电解质溶剂中的电泳运动实现了全彩色的动态等离激元显示。等离激元纳米结构的响应光谱和运动行为均可通过模拟计算事先得出以辅助结构与运动控制的参数设计。基于模拟计算的结果，实验中可以较容易地实现了等离激元电泳显示器件。这种等离激元动态彩色显示器件具有高对比度、高饱和度，并且可以可逆地运行多个周期。这是迄今为止实验上首次实现基于胶体等离激元金属纳米晶的电泳彩色显示器件。这一工作将有助于消除等离激元彩色显示器件进一步商业化的障碍。制造的等离激元电子“墨水”还可以应用于各种全纳米晶电子设备以及与颜色相关的工业品。

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[1] L. Shao, X. L. Zhuo, J. F. Wang*, "Advanced plasmonic materials for dynamic color display", Adv. Mater. 30: 1704338 (2018).

[2] J. P. Zheng, T. H. Chow, S. S. Li, J. F. Wang, L. Shao*, "Electrophoretic plasmonic ink for dynamic color display", Adv. Opt. Mater. 9: 2100091 (2021).

◀ 图 1　动态控制等离激元金属纳米晶颗粒的运动从而构筑电泳式彩色显示器件

CONTROL OF LIGHT-VALLEY INTERACTIONS IN 2D TRANSITION METAL DICHALCOGENIDES WITH NANOPHOTONIC STRUCTURES

(By **Shasha Li**, **Hao Wang**, **Jing Wang**, Huanjun Chen, **Lei Shao**)

Two-dimensional transition-metal dichalcogenides (2D TMDCs) possess unique valley properties and allow the robust manipulation of the valley degree of freedom via external fields. They show high potential for constructing high-performance optoelectronic and valleytronic devices. The related research has gained enormous interests. Despite the exciting progress in this field, manipulating the valley pseudospin is still challenging especially at room temperature because of the fast intervalley scattering. Integrating TMDCs with nanophotonic structures have been studied to address this challenge. Here, the nanophotonic approaches to facilitate the manipulation of the valley polarization are reviewed, including the valley-polarized photoluminescence mediated by surface plasmon resonance, the valley-polarized plasmon/photon–exciton polaritons generated through strong coupling, the spatial separation of valley polarized information by nanophotonic modes, and the valley polarization of excitons or carriers achieved by plasmon-enabled hot carrier injection. First, chiral plasmonic nanostructures have been used to enhance both the excitation and the spontaneous decay rate of the valley excitons, leading to improved valley contrast at room temperature even under the linearly polarized excitation. Second, strong coupling between photonic modes and the valley excitons offers another important approach to increase the valley polarization because of the long valley lifetime of the photonic part of the exciton-polaritons. Third, nanophotonic structures provide a useful platform for spatially routing the valley emission, which is promising for transporting and reading the valley pseudospin at the on-chip level. Moreover, the valley-selective injection of plasmon-induced hot carriers opens a new path for controlling the valley pseudospin. This review has highlighted the important research progress in the above fields. Open questions, major challenges, and interesting future developments in manipulating the valley information in 2D semiconductors with the help of nanophotonic structures are also discussed.

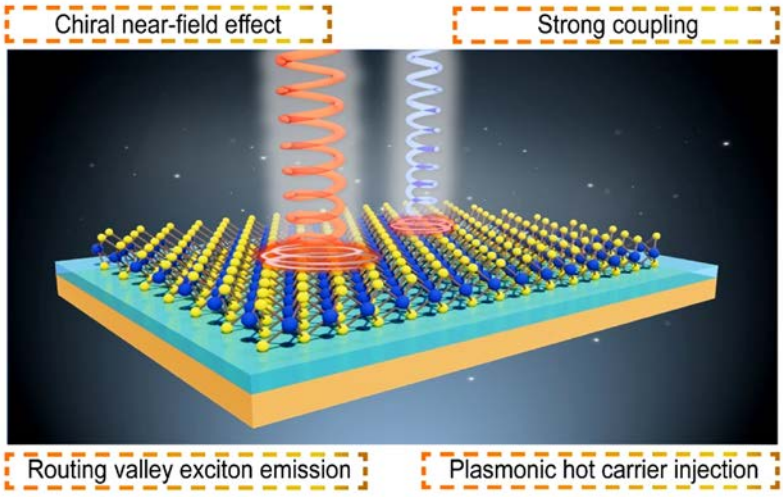

Fig. 1. Different physical mechanism for the control of light-valley interactions in 2D TMDCs with plasmonic nanostructures.

由纳米光子学结构调制的光场与二维过渡金属硫族化合物中电子能谷相互作用

（李莎莎，汪浩，王晶，陈焕君，邵磊）

二维过渡金属二硫属化物(2D TMDCs)具有独特的能谷赝自旋特性。这一能谷特性可以通过外场进行操纵，因此有潜力用于构建高性能的光电和能谷电子器件。相关研究方兴未艾。尽管如此，由于能谷间的快速散射过程，在室温下保留能谷信息并对其进行处理仍颇具挑战。通过将纳米光子学结构与2D TMDCs进行集成有希望应对上述挑战。本综述回顾了近来上述领域的研究进展。操纵能谷极化的纳米光子学方法包括利用表面等离激元近场调制光致发光的能谷极化、利用光场与激子的强耦合诱导产生能谷极化的极化激元、利用特定的纳米光子学模式实现能谷极化荧光的空间分离、以及利用等离激元热载流子实现激子或载流子的能谷选择性注入。首先，手性纳米结构的等离激元近场可被用于增强不同能谷激子的激发和自发衰减速率，从而在线偏振光激发下也能提高室温下的荧光能谷极化率。其次，由于等离激元(光子)/激子极化激元的光子部分的寿命较长，其可以长时间保存能谷极化信息，因而光场和能谷激子之间的强耦合也可提高能谷极化率。第三，自旋-动量锁定的纳米光子学模式可以使不同能谷辐射荧光在空间上分离，这有望在芯片级器件上实现能谷赝自旋的传输和读取。此外，等离激元热载流子的能谷选择性注入为控制能谷赝自旋开辟了一条新途径。这篇综述重点介绍了上述领域的重要研究进展，并且讨论了纳米光子学结构用于辅助操纵二维半导体中能谷信息这一领域的未解问题、主要挑战和未来发展。

◀ 图 1　利用等离激元结构调制光场与二维过渡金属硫族化合物中电子能谷相互作用的不同机制。

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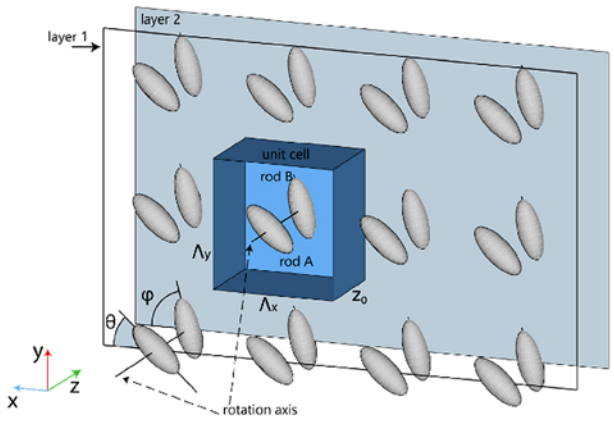
[1] S. S. Li, H. Wang, J. Wang, H. J. Chen, L. Shao*, "Control of light–valley interactions in 2D transition metal dichalcogenides with nanophotonic structures", Nanoscale 13: 6357-6372 (2021).

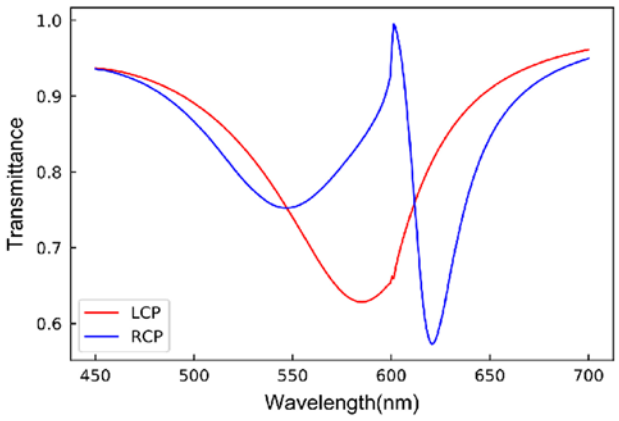
CHIRALITY-SELECTIVE TRANSPARENCY INDUCED BY LATTICE RESONANCE IN BILAYER METASURFACES

(By Shuxia Zhao, **Lei Shao**, Jianfang Wang, **Hai-Qing Lin**, **Wei Zhang**)

Chirality is of great importance in fundamental science, material design, biomedicine, and so on. Chiral optics associated with natural chiral molecules is limited by the fixed geometrical structure and weak optical signal mainly in the ultraviolet (UV) range. Plasmonic clusters supporting localized surface plasmon resonances (LSPRs) interact with visible light strongly, which can be controlled by the shape, size, position, and permittivity of the objects. Plasmonic nanostructures can be precisely designed with complex geometric patterns and thus provide many opportunities for exploring light–matter/structure interaction, in particular the chiral nature of photonics. Collective effects {such as lattice resonance (LR)} and interference effects (such as Fano resonance and electromagnetic induced transparency) modulated by electromagnetic (EM) field phase play important roles in controlling the optical properties. However, the study of the combination of those effects in the chiral metasurface area is in the preliminary stage. Many important issues need systematic studies.

This work theoretically explored the chiral optics of bilayer metasurfaces made of twisted nanorods, focusing on the collective effect due to LR. Through detailed analytical calculation based on CDM and FDTD simulations, it was found that combination effects from LR and phase modulation (PB phase, propagation phase) can bring about novel chiral optical responses, including chirality-selective transparency (recovery of Wood's anomaly) and chiral response for metasurfaces with achiral unit cells. The theoretical results deepen the understanding of light–matter interaction at the nanometer scale. In particular, the analytical results (supported by numerical simulation) give a quantitative relationship between local geometric structure, lattice structure, and their (chiral) optical properties. Those special properties of metasurfaces could play important roles in optical communication, circular dichroism spectroscopy, and quantum information processing.





双层银纳米棒超表面晶格共振诱导手性选择透明

(赵书侠，**邵磊**，王建方，**林海青**，张伟)

手性性质在基础科学、材料设计、生物医学等领域具有重要意义。天然手性分子的手性光学性质受其几何结构参数限制，大多没有很强的手性光学响应，且其响应主要在紫外波段。具有局域表面等离激元共振特性(LSPR)的金属纳米结构可以与可见光发生较强的相互作用，其光学响应可通过调控物体的形状、大小、位置和介电常数来控制。因而，设计成特定几何图案的等离激元纳米结构为探索光-物质相互作用提供了更多可能，也为增强结构的手性光学响应提供了新的载体。特别是，由电磁场相位调制的集体效应(例如晶格共振LR)和干涉效应(例如Fano共振和电磁感应透明)在控制结构的光学响应方面起着重要作用。然而，这些效应在手性超表面结构中作用尚待进一步探索，许多重要问题需要系统研究。本工作从理论上探索了扭曲银纳米棒双层超表面的手性光学性质，重点关注LR引起的集体效应。基于CDM和FDTD模拟的详细计算分析表明，LR和相位调制(PB相位、传播相位)的共同作用可以带来新的手性光学响应，尤其是手性选择性透明，并且可以利用非手性晶胞超表面实现手性光学响应。这些结果加深了人们对纳米尺度下光与物质相互作用的理解。特别是，本工作给出了局域几何结构、晶格结构及其手性光学特性之间的定量关系。本工作报道的具有特殊手性性质的光学超表面预期在光通信、圆二色光谱和量子信息处理中发挥重要作用。

References:

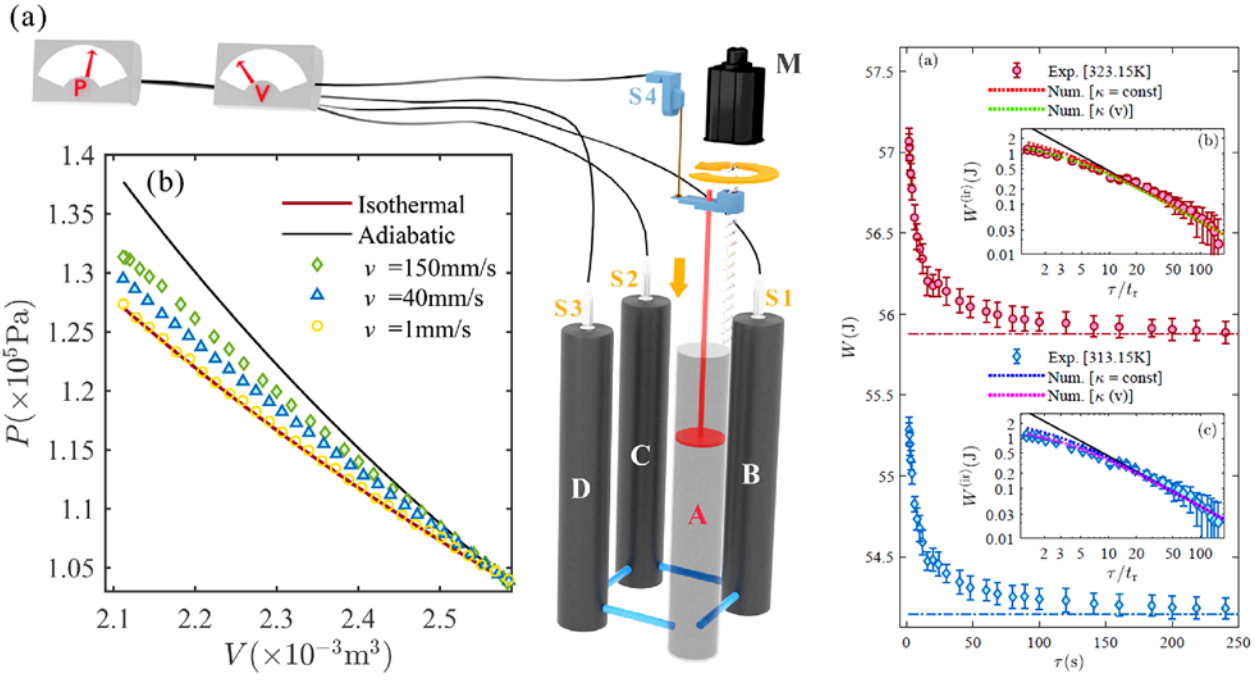
[1] S.-X. Zhao, L. Shao, J. F. Wang, H.-Q. Lin*, W. Zhang*, "Chirality selective transparency induced by lattice resonance in bilayer metasurfaces", *Photonics Res*. 9: 484-493 (2021).

EXPERIMENTAL TEST OF THE 1/T-SCALING ENTROPY GENERATION IN FINITE-TIME THERMODYNAMICS

(By **Yu-Han Ma**, Ruo-Xun Zhai, **Jinfu Chen**, **C. P. Sun**, and Hui Dong*)

The finite-time dynamics, apart from its fundamental importance in nonequilibrium thermodynamics, is of great significance in designing heat engine cycles. We build an experimental apparatus to test the predicted long-time $1=\tau$ scaling of the irreversible entropy generation in the finite-time (τ) thermodynamic process by compressing dry air in a temperature-controlled water bath. We present the first direct experimental validation of the scaling, utilized in many finite-time thermodynamic models at the long-time regime. The experimental data also demonstrate a clear deviation from the scaling at the short-time regime. We show the optimal control scheme to minimize the irreversible entropy generation in finite-time process. Such optimization shall bring new insight to the practical design of heat engine cycles.

The research group led by Professor Sun Chang-Pu of Beijing computing science research center and Associate Professor Dong Hui of Graduate School of Chinese Academy of physics has completed the research of this work, and the relevant achievement is “Experimental Test of the 1/τ-Scaling Entropy Generation in Finite-Time Thermodynamics” was published in *Physical Review Letters* (125, 210601, 2020) in November 2020.



有限时间热力学中不可逆熵产生时间反比律的实验验证

（马宇翰，翟若迅，陈劲夫，孙昌璞，董辉）

有限时间热力学的发展使得人们开始在理论上研究更接近现实的实际热机：在偏离准静态假设的有限时间的热力学循环中运行的热机。热力学第二定律指出热机在经历这样的热力学循环后会有不可逆的熵增。在不同模型和系统中的理论研究都表明，在有限时间等温过程中，不可逆熵产生在长时区域与过程时间恰好成反比。作为非平衡热力学中为数不多的定量关系，这一熵增的时间反比律被广泛用于不同热力学过程及循环的优化中。然而，我们注意到，一直以来都缺乏对这一关系定量的实验研究。

在这项工作中，我们设计并搭建了一个基于理想气体的实验平台，通过在控温水浴环中压缩干燥空气，首次验证有限时间热力学过程(过程时间为 τ)中不可逆熵产生在长时区域的1/ τ 标度行为。我们的实验结果还表明，在短时区域熵产生会明显偏离长时区的1/ τ 标度。 此外，本研究展示了一种最优控制方案，可以最大限度地减少有限时间过程中的不可逆熵产生。 这种优化将为实际热机循环的设计提供新的视角。

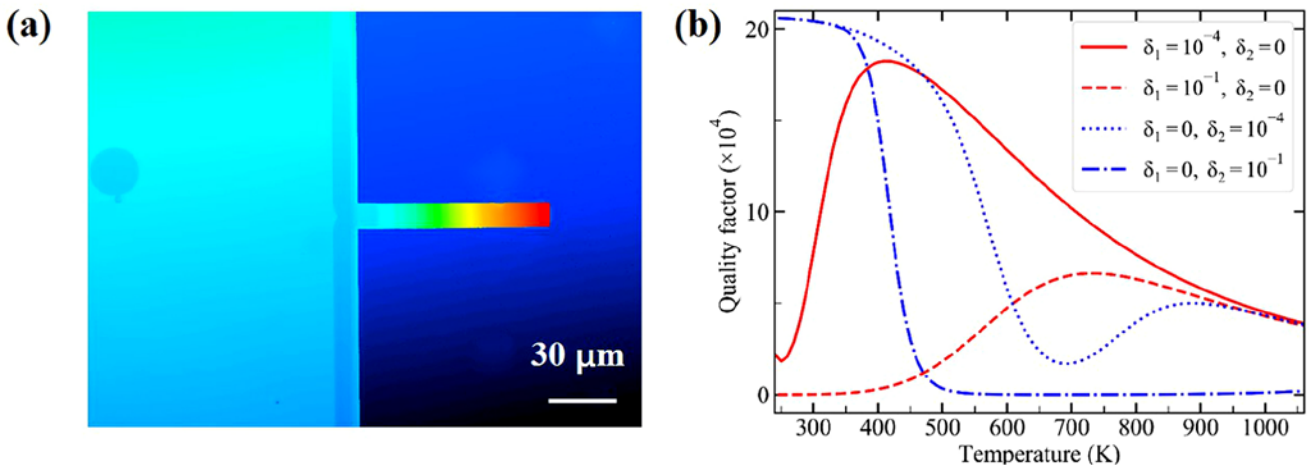
北京计算科学研究中心的孙昌璞教授和中物院研究生院董辉研究员领导的课题组完成了该项工作的研究，相关成果《Experimental Test of the 1/ τ -Scaling Entropy Generation in Finite-Time Thermodynamics》于2020年11月发表在《*Physical Review Letters*》(125, 210601 2020)上。

EFFECT OF DEEP-DEFECTS EXCITATION ON MECHANICAL ENERGY DISSIPATION OF SINGLE-CRYSTAL DIAMOND

(By **Huanying Sun**, Liwen Sang, Haihua Wu, Zilong Zhang, Tokuyuki Teraji, Tie-Fu Li, J. Q. You, Masaya Toda, Satoshi Koizumi, and Meiyong Liao*)

The ultrawide band gap of diamond distinguishes it from other semiconductors, in that all known defects have deep energy levels that are less active at room temperature. Here, we present the effect of deep defects on the mechanical energy dissipation of single-crystal diamond experimentally and theoretically up to 973 K. Energy dissipation is found to increase with temperature and exhibits local maxima due to the interaction between phonons and deep defects activated at specific temperatures. A two-level model with deep energies is proposed to explain well the energy dissipation at elevated temperatures. It is evident that the removal of boron impurities can substantially increase the quality factor of room-temperature diamond mechanical resonators. The deep energy nature of the defects bestows single-crystal diamond with outstanding low intrinsic energy dissipation in mechanical resonators at room temperature or above.

For more details, please refer to the original paper of *Physical Review Letters* published online (DOI: 10.1103 / Physical Review letter. 125.206802). Sun Huan-Ying is the first author of the paper.



单晶金刚石机械能耗的深能级效应

（**孙换莹**，桑立雯，吴海华，张子龙，Tokuyuki Teraji，李铁夫，游建强，Masaya Toda，Satoshi Koizumi，廖梅勇*）

微机电系统（MEMS）是通过微纳加工技术将微机械结构、微传感器、微执行器、微电源、信号处理和控制电路、通信等集成于一体的微型器件或系统。与其他传感器相比，MEMS传感器具有多功能、体积小、重量轻、功耗低、高精度和易量产等优点，可广泛应用于消费电子、汽车工业、通信、航空航天、医疗诊断以及科学研究等领域，如加速度计、陀螺仪、射频开关、麦克风、微投影仪、压力传感器、气体传感器、质量分析仪、扫描显微镜探针等，是物联网和智能社会的变革性技术。

困扰MEMS的主要问题是同时满足器件的稳定性、可靠性以及高性能。金刚石具有5.5 eV的超宽带隙，并且具有最高的硬度和弹性常数、最高的热导率，是理想的高可靠性MEMS材料。但金刚石的MEMS应用受制于单晶金刚石的加工难等课题。该小组于2010年，提出全单晶金刚石MEMS的基本概念，利用智能剪切技术，实现了单晶金刚石微纳机械结构形状和尺寸的可控加工，成功研制出第一个真正意义上的单晶金刚石MEMS器件，开创了单晶金刚石MEMS领域(Liao et al, Adv. Mater. 22,5393，2010)。该小组2018年又成功研制出品质因子(Q)超百万的金刚石悬臂梁谐振子(H.Wu et al, Phys. Rev. Mater. 2, 090601(R)，2018)，并同时将电信号驱动和传感集成于同一金刚石衬底。

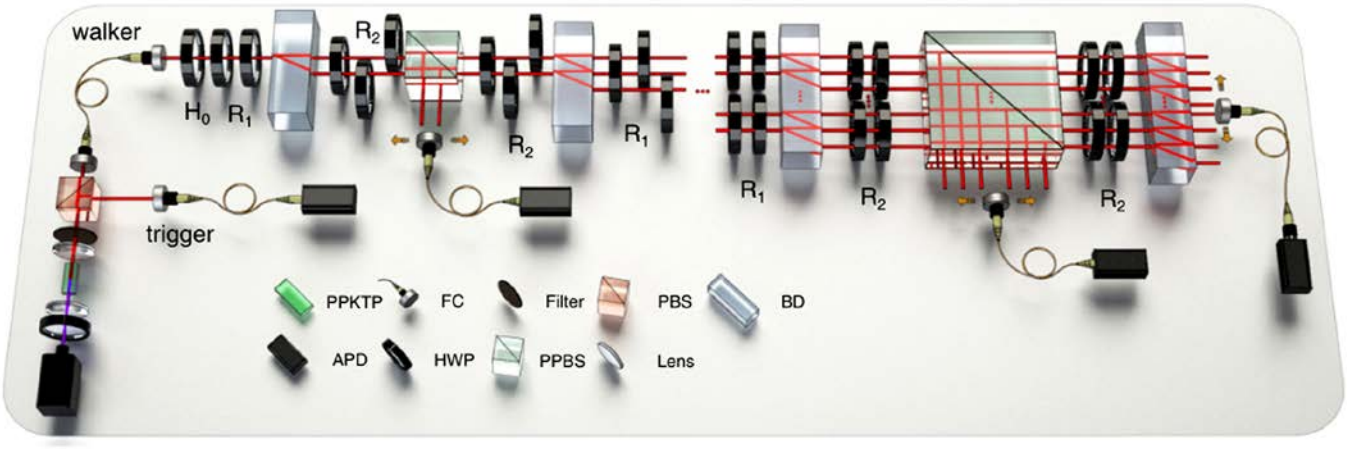
最近，该小组从实验和理论上研究了深能级缺陷对单晶金刚石机械能耗的影响。研究发现，从室温到700摄氏度，金刚石的机械能耗散随温度升高而增加，但由于声子与深能级缺陷之间的相互作用而表现出局部最大值。研究发现除去硼杂质可以显著提高谐振子的Q值，而金刚石中常见的氮杂质具有很高的激活能，只有在高温下才对机械能耗有贡献。本研究从深能级缺陷的新角度，表明单晶金刚石优于其他半导体材料，是高灵敏度、高稳定性和高可靠性MEMS的理想材料。传统半导体如Si，GaAs，SiC和III族氮化物，浅能级掺杂对于半导体器件是必需的，而深能级杂质通常会降低半导体器件的性能。金刚石作为超宽带隙半导体，目前已知的体掺杂都具有深能级，限制了其作为半导体器件的应用。然而，廖梅勇研究小组从实验和理论上证明了金刚石中的深能级缺陷效应反而使其在MEMS领域具有其他半导体材料无法比拟的优势，即金刚石具有更小的机械能耗，可以获得更高品质因子的机械谐振子，有利于实现更高灵敏度的MEMS传感器。更多细节可以参考在线发表的Physical Review Letters的原论文(DOI：10.1103/PhysRevLett.125.206802)，博士生孙换莹为论文的第一作者。该研究得到日本文部省科研费(20H02212, 15H03999)以及中国国家留学基金委公派研究生项目的资助。

OBSERVATION OF NON-BLOCH PARITY-TIME SYMMETRY AND EXCEPTIONAL POINTS

(By **L. Xiao**, T. S. Deng, **K. K. Wang**, Z. Wang*, W. Yi*, and **P. Xue***)

Parity-time (PT)-symmetric Hamiltonians have widespread significance in non-Hermitian physics. A PT-symmetric Hamiltonian can exhibit distinct phases with either real or complex eigenspectrum, while the transition points in between, the so-called exceptional points, give rise to a host of critical behaviors that holds great promise for applications. For spatially periodic non-Hermitian systems, PT symmetries are commonly characterized and observed in line with the Bloch band theory, with exceptional points dwelling in the Brillouin zone. Here, in nonunitary quantum walks of single photons, we uncover a novel family of exceptional points beyond this common wisdom. These "non-Bloch exceptional points" originate from the accumulation of bulk eigenstates near boundaries, known as the non-Hermitian skin effect, and inhabit a generalized Brillouin zone. Our finding opens the avenue toward a generalized PT-symmetry framework, and reveals the intriguing interplay between PT symmetry and non-Hermitian skin effect. In view of the potential utilities of exceptional points, the non-Bloch exceptional points observed here would inspire novel designs and applications such as enhanced sensing with interface-sensitive, ultrahigh spatial resolutions, or robust wireless power transfer that are tunable by the interface geometry.

Recently, the research team led by Prof. Peng Xue at Beijing Computational Science Research Center, reported an experiment on observation of non-Bloch prity-time symmetry and exceptional points was published *Physical Review Letters* (126, 230402 2021).



非布洛赫宇称–时间对称和临界点的实验观测

(肖磊，邓天舒，王坤坤，汪忠*，易为*，薛鹏*)

具有宇称-时间对称的系统在非厄米物理中具有广泛应用。满足宇称-时间对称的非厄米系统具有对称保持相和对称破缺相，两相由奇异点分隔，其中对称保持相拥有纯实本征能谱，而对称破缺相具有复数能谱。宇称-时间对称体系具有一系列独特的物理性质，此外奇异点附近的临界行为在精密测量等方面具有应用前景。在凝聚态物理、光子晶体等多个领域中，具有空间周期结构的体系一般纳入布洛赫(Bloch)能带理论的框架下描述，奇异点存在于布里渊区中。

这里，我们用单光子的离散时间量子行走观测到一类奇特的奇异点，和布洛赫能带理论不同，这类奇异点不能用布洛赫能带理论描述，取而代之的是非布洛赫理论。这类“非布洛赫奇异点”起源于全部体本征态都局域在边界的非厄米趋肤效应，可以适用于基于广义布里渊区建立的非布洛赫理论。我们的研究开辟了对广义宇称-时间对称的研究，并且揭示了宇称-时间对称和非厄米趋肤效应的相互联系。非布洛赫奇异点的研究在高精度传感和无线能量传输方面都有着广泛的潜在应用前景。

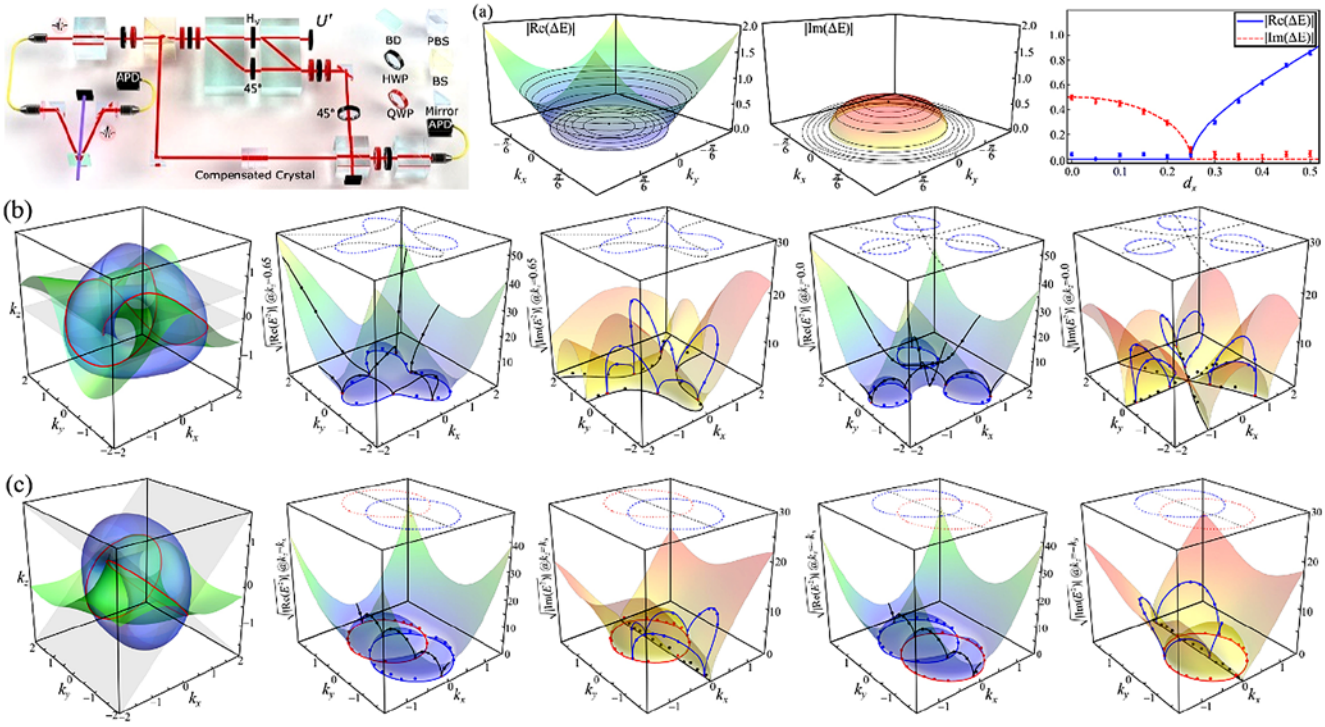
北京计算科学研究中心的薛鹏教授领导的课题组完成了该项工作的研究，相关成果《Observation of Non-Bloch Parity-Time Symmetry and Exceptional Points》于2021年6月发表在《*Physical Review Letters*》(126, 230402 2021)上。

SIMULATING EXCEPTIONAL NON-HERMITIAN METALS WITH SINGLE-PHOTON INTERFEROMETRY

(By **Kunkun Wang**, **Lei Xiao**, Jan Carl Budich*, W. Yi*, and **P. Xue***)

Recently, it has become clear that non-Hermiticity, a common element in open, dissipative systems, can qualitatively modify the phases of quantum matter characterized by topologically robust nodal band structures. Here, we experimentally simulate in a photonic setting non-Hermitian metal characterized by the topological properties of their nodal band structures. Implementing nonunitary time evolution in reciprocal space followed by interferometric measurements, we probe the complex eigenenergies of the corresponding non-Hermitian Bloch Hamiltonians, and study in detail the topology of their exceptional lines, the non-Hermitian counterpart of nodal lines in Hermitian systems. We focus on two distinct types of non-Hermitian metals: two dimensional systems with symmetry-protected exceptional lines, and three-dimensional systems possessing symmetry independent topological exceptional lines in the form of knots. While both types feature open Fermi surfaces, we experimentally observe their distinctions by analyzing the impact of symmetry-breaking perturbations on the topology of exceptional lines.

Recently, the research team led by Prof. Peng Xue at Beijing Computational Science Research Center, reported an experiment on simulating exceptional non-Hermitian metals with single-photon interferometry, which was published in *Physical Review Letters* (2021, **127**, 026404).



单光子干涉仪模拟奇异非厄米金属

（王坤坤，肖磊，Jan Carl Budich*，易为，薛鹏*）

近年来，诸多研究表明，普遍存在于开放耗散系统中的非厄米性，可以改变系统拓扑能带结构，丰富量子材料中的拓扑相，引发系统中许多的奇特效应。通过采用单光子偏振态编码动量空间中非厄米金属能级，将动量编码于玻片角度，再引入光子数丢失，我们实验模拟了相应非厄米金属对应哈密顿量演化，并采用干涉测量，实现了对非厄米哈密顿量复本征能量的测量，进而实现了对非厄米金属能带中奇异线结构完整的模拟和刻画。实验中，通过调整玻片角度，分别模拟了两种不同的非厄米金属能带结构。在第一种非厄米金属中，通过引入对称性，降低了系统中奇异线的存在对系统维度的要求，实验观测到了二维系统中对称保护的奇异线能带结构；在第二种三维非厄米金属中，分别观测到了不依赖于对称性的结式和链式奇异线能带结构；实验在两种金属结构中均观测到了费米面的存在。在此基础上，还研究了两种非厄米金属中奇异线结构在不同微扰下的稳定性。结果表明，对于二维空间中对称保护的奇异线结构，在微小的对称破缺的微扰下，奇异线消失，而在对称性保持的微扰下，奇异线的存在具有鲁棒性，而对于三维空间中的结式和链式奇异线能带结构，即使是在能够破坏所有对称性的随机微扰下，其特殊能带结构也呈现出一定稳定性。

北京计算科学研究中心的薛鹏教授领导的课题组完成了该项工作的研究，相关成果以《Simulating Exceptional Non-Hermitian Metals with Single-Photon Interferometry》为题，于2021年7月发表在《物理评论快报》上。

SPATIAL ENANTIOSEPARATION OF GASEOUS CHIRAL MOLECULES

(By **By Bo Liu**, **Chong Ye, C. P. Sun**, and **Yong Li**)

The study of chiral molecules is fundamentally significant in organic chemistry, pharmacology, biochemistry, as well as atomic, molecular, and optical physics. Cyclic three-level models [1-5] formed by applying three electromagnetic fields to couple with the electric dipole transitions among three levels play an important role in the studies of chiral molecules. In such a cyclic three-level model, the product of the three corresponding coupling strengths of the electric dipole transition moments changes sign with enantiomers. Then the overall phase of the product of the three corresponding coupling strengths differs by π with enantiomers, which can be used to realize inner-state enantioseparation [1], spatial enantioseparation [2], and enantiodetection [3].

In these previous theoretical works of chiral molecules [2], molecular rotations were not involved. For real gaseous chiral molecules, the molecular rotations should be considered. Due to the magnetic degeneracy of the molecular rotational states, only three electromagnetic fields with appropriate polarization vectors and frequencies can construct the cyclic three-level configuration for gaseous asymmetric-top chiral molecules [4,5]. Then the propagation directions of three electromagnetic fields may not be parallel. Under the three-photon resonance condition, molecules in different spatial positions experience different space-dependent parts of the overall phases of the coupling strengths, which results in the problem of phase mismatching in the enantioseparation and the enantiodetection.

Here, we explore the center-of-mass motion of gaseous chiral molecules under induced gauge potentials, and find that the space-dependent part of the overall phase (besides the spatial distribution of the intensity of the three coupling strengths, similar to previous work of spatial enantioseparation [2]) offers an additional resource that results in induced gauge potentials. Under the induced gauge potentials resulting from the space-dependent part of the overall phase and the space-dependent intensities of coupling strengths, we further show the obvious spatial enantioseparation for typical parameters of gaseous chiral molecules (see the following figure).
For more information, please see the paper B. Liu, C. Ye, C. P. Sun, and Y. Li, *Phys. Rev*. A **104**. 013113 (2021).

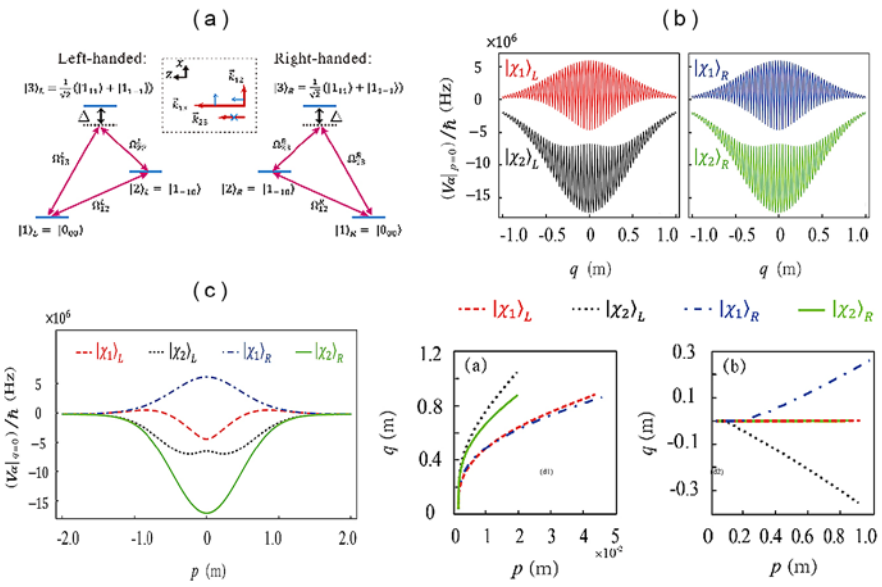


Fig. 1. (a) Model of cyclic three-level gaseous chiral molecules. (b) Induced scalar potentials V_α at fixed $p = 0$ in the $\hat{q}$ direction and (c) induced scalar potentials V_α at fixed $q = 0$ in the $\hat{p}$ direction corresponding to enantiomers with different inner dressed states. Propagation trajectories of the chiral molecules with initial velocity (d1) in the $\hat{q}$ direction or (d2) in the $\hat{p}$ direction.

气态手性分子的空间分离

（刘博，叶冲，孙昌璞，李勇）

手性分子的研究在有机化学、药理学、生物化学以及原子、分子和光学物理中具有重要意义。在手性分子的研究中，外加三个电磁场分别耦合三个能级间的电偶极跃迁而形成的循环三能级模型[1-5]起着重要的作用。在手性分子的循环三能级模型中，三个耦合系数的乘积依赖于手性，即其总相位相差 ，利用该相位差可实现左右手性分子的内态分离[1]、空间分离[2]和手性探测[3]。

先前的手性分子的理论工作通常忽略了分子的转动[2]。然而，对于实际的气态手性分子，应该考虑分子的转动。由于分子转动态的磁量子数简并，只有选择合适的偏振方向和频率的三个电磁场才能构成气态非对称陀螺型手性分子的循环三能级模型[4,5]。那么，三个电磁场的传播方向不可能彼此平行。因此，在三光子共振条件下，耦合系数整体相位将依赖于分子的空间位置，这导致了手性分子的内态分离和手性探测的相位不匹配问题。

我们的研究表明，这一整体相位的空间依赖部分（除了与先前空间分离工作[2]类似的三个耦合系数的强度的空间分布之外）提供的额外资源导致了诱导规范势。在耦合系数的空间依赖的强度和整体相位的空间依赖部分共同产生的诱导规范势下，我们进一步展示了气态手性分子在典型参数下显著的空间分离（见左图）。

更多相关信息，请参阅 B. Liu, C. Ye, C. P. Sun, and Y. Li, Phys. Rev. A **104**, 013113 (2021).

◀ 图 1　气态手性分子的循环三能级模型 (a)。手性异构体的不同内部缀饰态在$p = 0$ 处沿 $\hat{q}$ 方向的诱导规范标势 V_α (b) 和在 $q = 0$ 处沿 $\hat{p}$ 方向的诱导规范标势 V_α (c)。初速度沿 $\hat{q}$ 方向 (d1) 和沿 $\hat{p}$ 方向 (d2) 的手性分子运动轨迹。

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[2] Y. Li, C. Bruder, and C. P. Sun, Phys. Rev. Lett. **99**, 130403 (2007).
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ORIGIN OF IRRADIATION SYNERGISTIC EFFECTS IN SILICON BIPOLAR TRANSISTORS

(By Yu Song* and **Su-Huai Wei***)

Si-based NPN and PNP transistors are building blocks of modern microelectronics, such as operational amplifiers and voltage comparators. When these devices are used in outer space and other extreme environments such as nuclear reactors, both charge carriers and atomic displacements will be generated in the silica and silicon materials, which result in ionization and displacement damages in the devices. Conventionally, the practical damage is usually assumed as a simple sum of the ionization damage (ID) and displacement damage (DD), which then can be evaluated individually at ground by carrying out γ-ray and neutron irradiation experiments, respectively.

Recent experiments show a clear difference between the practical and summed damages of silicon bipolar devices subjected to mixed ionization and displacement irradiations, indicating significant irradiation synergistic effects (ISEs). Previous models attribute the effect to a Coulomb interaction of oxide trapped charges in silica on charge carriers in irradiated silicon, however, it encounter difficulty to understand the dose-rate dependence of the ISEs. In this work [1], we propose that an ionization-induced evolution of displacement defects should be responsible for this basic phenomenon. Specifically, for the negative ISE observed in PNP transistors, we propose an atomistic model of transformation and annihilation of displacement-irradiation-induced V2 and VO defects in n-type silicon under ionization irradiation. Based on which we derived a model for the dose and fluence dependence of the base current. The predicted novel dose and fluence dependences are fully verified by the experimental data. Our work uncovers the essential role of ionization irradiation played in the evolution of displacement defects; it can be used to predict the practical damages of semiconductor devices in mixed ionization and displacement irradiations.

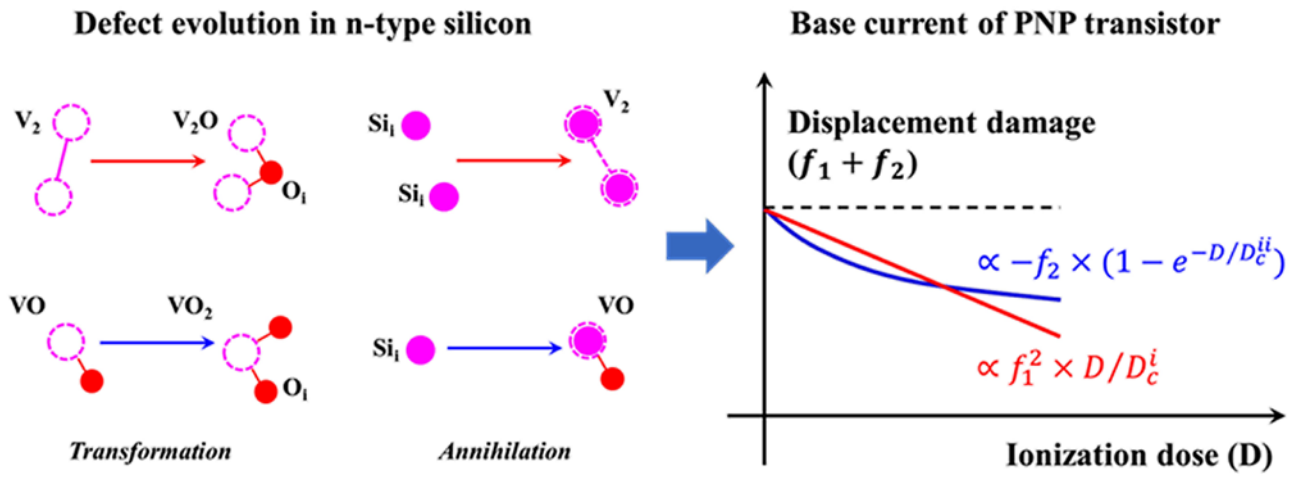

Fig. 1. Ionizing-irradiation-induced defect evolution in n-type silicon (left column) as the origin of the synergistic effect observed in neutron- and gamma-ray-irradiated PNP transistors (right column).

硅双极晶体管中辐照协同效应的物理起源

（宋宇*，**魏苏淮***）

基于硅的 NPN 和 PNP 晶体管是现代微电子器件中的基础器件，例如运算放大器和电压比较器等。当这些器件用于外太空和其他极端环境（如核反应堆）时，二氧化硅和硅材料中会产生电荷载流子和原子位移，从而导致器件发生电离和位移损伤。通常，实际损伤通常被假设为电离损伤（ID）和位移损伤（DD）的简单总和，然后可以通过分别在地面进行 γ 射线和中子辐照实验来单独评估。

最近的实验研究表明，处于电离和位移复合辐照环境中的硅双极晶体管表现出非常不同于单独损伤之和的实际损伤，意味着存在显著的辐照协同效应。以往的模型将该效应归结于晶体管中氧化物陷阱电荷对硅沟道载流子的库仑相互作用，但无法解释协同效应随剂量率降低而增强的实验趋势。在本工作中[1]，我们提出了“电离诱导的位移缺陷演化”的全新物理机制。具体而言，对于PNP晶体管中负的协同效应，我们构建了n型硅中位移辐照诱导V2和VO缺陷在电离辐照下的转化和湮灭动力学模型，以及对应的晶体管基极电流损伤模型。后者预测的新奇的电离剂量依赖性和位移注量依赖性被实验完全证实。该工作揭示了电离辐照对位移缺陷的重要作用，可以用于预测复杂辐照环境下半导体器件的实际损伤。

◀ 图 1　位移-电离辐照PNP晶体管中的协同效应（右）起源于n型硅中电离辐照诱导的位移缺陷演化（左）。

References:

[1] Y. Song* and S.-H. Wei*, ACS Appl. Electron. Mater. 2, 3783 (2020). (As *Spotlight on Applications*)

BROADBAND DIRAC PLASMONS IN BOROPHENE

(By Chao Lian, Shiqi Hu, Jin Zhang, Cai Cheng, Zhe Yuan, **Shiwu Gao*** and Sheng Meng*)

Propagating surface plasmons with broad frequency tunability and low loss rate are promising for optoelectronic applications and quantum information processing. Noble metal thin films can sustain high-frequency plasmon waves due to the free electrons. However, they generally suffer from low spatial confinement and significant energy losses during propagation, due to the manifold interband transitions and strong coupling to phonons. Ultra-thin films like graphene have low loss surface plasmons due to the suppression of Landau damping. However, the frequency of the graphene plasmons is in the far-infrared regime and is hardly tunable. Therefore, 2D materials with higher carrier density and higher plasmon frequencies are particularly desirable for fundamental research and optoelectronic applications.

Recent study of surface plasmon in borophene, a single layer of boron metal, suggests that their surface plasmons have very unique properties with broad band dispersion, highly spatial confinement, and strong anisotropy in momentum space [1]. Due to the much higher free electron density, the Dirac plasmon of borophene have two branches whose energy extends to the visible regime. In addition, these plasmons have much stronger spatial confinement and show strong anisotropy in momentum space, which is promising for directional control of wave propagation. These conclusions are obtained by accurate linear response calculation based on time-dependent density functional theory (LR-TDDFT), together with simple model analysis, which were carried out by joint collaboration between CSRC (Shiwu Gao) and Institute of Physics (Sheng Meng), Chinese Academy of Sciences.

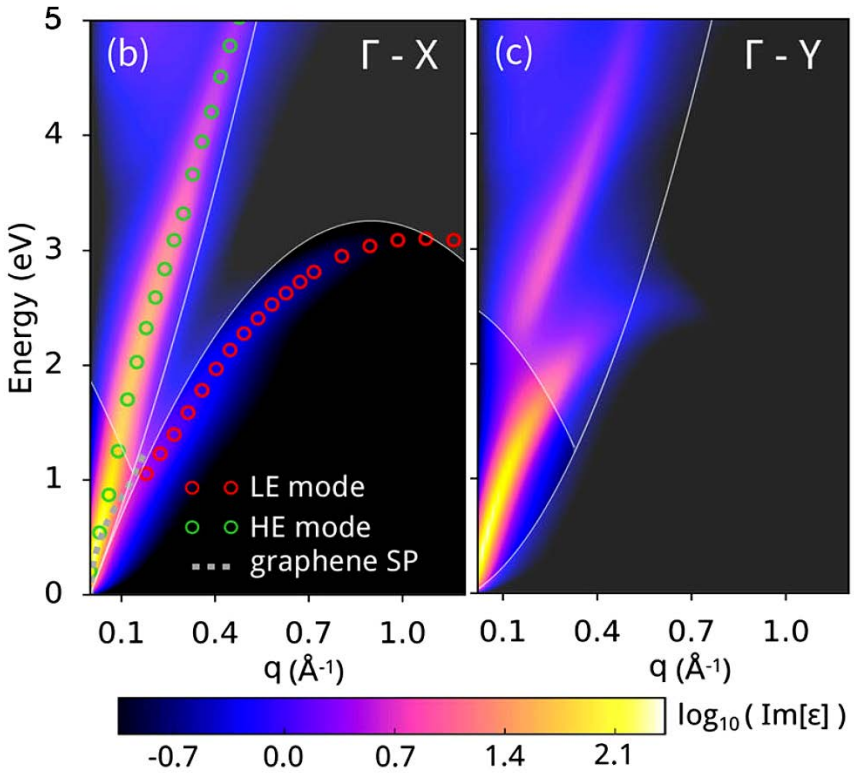

Fig. 1. The low-energy (LE) and high energy branch (HE) of the Dirac plasmon for borophene, which shows strong anisotropy and broad band dispersions.

硼烯中的宽带等离激元的理论预测

(廉超，胡史奇，张进，陈才，袁喆，**高世武***，孟胜*)

具有宽频率可调性和低损耗率的表面等离激元，在光电应用和量子信息处理中具有广阔的应用前景。由于自由电子的存在，贵金属薄膜可以产生高频等离激元波。然而，由于多重带间跃迁和与声子的强耦合损耗，它们在传输过程中通常会受到较低的空间限制和较大的能量损失。超薄的二维材料如石墨烯具有低损耗的表面等离激元。但是，石墨烯等离激元的频率主要处于远红外区，且很难调制。因此，具有更高载流子密度和更高等离激元频率的二维材料对于等离激元学的基础研究和光电器件应用都有需要的意义。

最近对硼单层膜（硼烯）的表面等离激元的研究表明，它们的表面等离激元具有非常独特的性质，包括宽带色散、高度空间限制和动量空间的超强各向异性[1]。与石墨烯不同，硼烯的狄拉克等离激元有两个分支，其高能一支能量可延伸到可见光区。这些等离激元具有更强的空间约束性，在动量空间表现出强烈的各向异性，这为等离激元波的传播方向控制带来了希望。这些结论是在基于含时密度泛函理论（LR-TDDFT）的线性响应计算和简单模型分析的基础上，由北京计算科学研究中心（高世武）和中国科学院物理研究所（孟胜研究组）合作研究进行的。

◀ 图 1　硼稀的狄拉克等离激元模式包括两支：低能模（LE）和高能模（HE）。他们显出很宽的能量色散关系和强烈的各向异性。

References:

[1] Chao Lian, Shi-Qi Hu, Jin Zhang, Cai Cheng, Zhe Yuan, Shiwu Gao*, and Sheng Meng*, Integrated plasmonics: Broadband Dirac plasmons in borophene, *Phys. Rev. Lett*. 125, 116802 (2020).

PREDICTION AND REGULATION OF METALLIC GLASS PROPERTIES BASED ON THE POTENTIAL ENERGY SURFACE INVESTIGATIONS

(By **Pengfei Guan**'s Group)

According to the basic conception of potential energy landscape (PEL), the properties of materials are determined by the basic features of their potential energy surface morphology. Therefore, the study of the properties of the potential energy surface of the amorphous alloy system is of great significance to understand the physical properties of the amorphous alloy material and its evolution in the external field. By combining molecular dynamics simulations, machine learning, and potential energy surface (PES) searching methods, we 1) provide direct evidence for the hierarchical characteristics of PES in bulk amorphous alloys, and establish a qualitative correlation between the hierarchical properties and the low-temperature relaxation peaks of amorphous alloys [1].The properties of the low temperature relaxation peak are closely related to the macroscopic mechanical properties of the amorphous alloy. 2) The microscopic mechanism of amorphous rejuvenation induced by thermal-cycling at low temperature [2] was clarified, providing a new idea for the regulation of the properties of amorphous alloys. 3) Based on the characteristics of the second derivative of the PES, the critical buckling stress of the "intrinsic defect" in different loading directions was defined, and an effective parameter for predicting the protocol-dependent response of shear transformation zone was proposed [3]. 4) The critical size effect of the PES of the amorphous alloy is revealed. The intrinsic properties of the flat potential energy surface of the amorphous nanoclusters (<100 atoms) are pointed out. This provides a theoretical basis for the performance design of the nano-amorphous [4, 5].

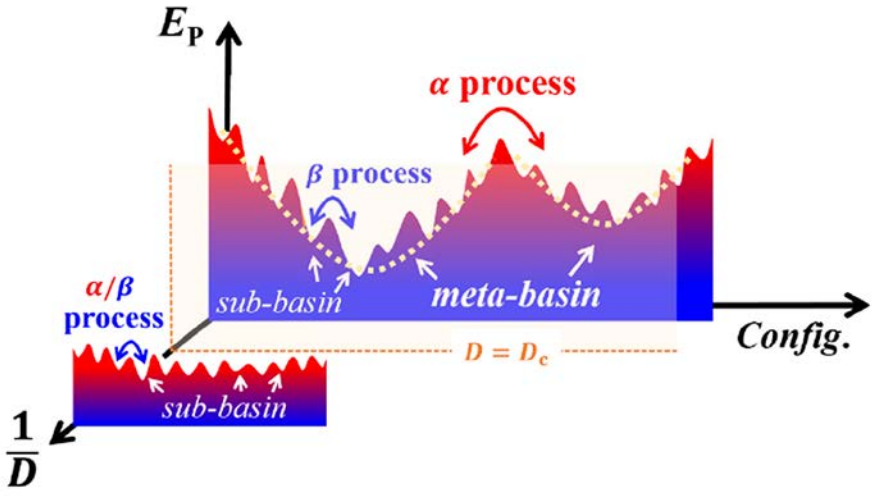

Fig. 1. The schematic diagram of PEL morphology with size reduction in configuration space.

基于势能曲面特性的非晶合金性能预测与调控

（管鹏飞课题组）

基于势能图景的基本框架，材料的性能由其势能曲面形貌的基本特征决定。因而，研究非晶合金体系势能曲面的特性对认识非晶合金材料的物性及其在外场下的演化具有重要的意义。基于分子动力学模拟，机器学习及势能面搜索方法，我们1）给出了块体非晶合金势能曲面层级特征的直接证据，并建立了其层级特性与非晶合金低温弛豫峰之间的定性关联[1]，这一低温弛豫峰的性质与非晶合金的宏观力学性能密切相关；2）阐明了低温冷热循环诱导非晶年轻化的微观机理[2]，为非晶合金性能调控提供了新思路；3）基于势能曲面二阶导的特征，定义了“本征缺陷”在不同加载方向的临界失稳应力，提出了预测局域塑性事件加载方向敏感性的有效参量[3]；4）发现了团簇非晶动力学行为的强-脆转变现象，揭示了非晶合金势能曲面特征的临界尺度效应，指出了平坦势能面是非晶纳米团簇(<100 atoms)的本征属性，为纳米非晶性能设计提供了理论基础[4,5]。应邀以“金属玻璃结构及其失稳的原子层次研究”为题撰写综述论文[6]。

基于针对复杂合金体系势能曲面研究的基础，运用机器学习算法，通过定义局域原子环境参量，实现了对复杂合金体系第一性原理势能曲面的高精度数值重建，并以此为基础完成高效大尺度分子动力学模拟，实现从量子力学计算到经典力学模拟的跨越，拓展了精确数值模拟的时空尺度，最终有望从电子层子关联材料的宏观物性及其演化，为面向院内的实际需求，开展针对材料辐照效应及活性金属腐蚀机理与性能预测的跨时空尺度模拟研究奠定了基础。

◀ 图 1　复杂合金体系势能曲面形貌的尺寸相关性示意图.

References:

[1] B. Wang, L. J. Wang, B. S. Shang, X. Q. Gao, Y. Yang*, H. Y. Bai, M. X. Pan*, W. H. Wang, P. F. Guan*, Revealing the low-temperature fast relaxation peak in a model metallic glass, *Acta Mater*. 195, 2611-620(2020).

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[4] S. J. Sun, P. F. Guan*. The critical model size for simulating the structure-dynamics correlation in bulk metallic glasses. *Sci. China Mater*., 64, 1545-1555(2021)

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UNIFIED THEORY FOR DENSITY-INDEPENDENT PLASMONS

(By **Bing Huang**'s Group)

To efficiently integrate cutting-edge terahertz technology into compact devices, the highly confined terahertz plasmons are attracting intensive attention. Compared to plasmons at visible frequencies in metals, terahertz plasmons, typically in lightly doped semiconductors or graphene, are sensitive to carrier density (n) and thus have an easy tunability, which leads to unstable or imprecise terahertz spectra. By deriving a simplified but universal form of plasmon frequencies, in their recent study, Bing Huang's Group reveal a unified mechanism for generating unusual n-independent plasmons (DIPs) in all quantum states with different dimensions. Remarkably, they predict that terahertz DIPs can be excited in a two-dimensional nodal line and one-dimensional nodal point systems, confirmed by their first-principles calculations on almost all existing topological semimetals with diverse lattice symmetries. Besides n-independence, the feature of Fermi velocity and degeneracy factor dependencies in DIPs can be applied to design topological superlattice and multiwalled carbon nanotube metamaterials for broadband terahertz spectroscopy and quantized terahertz plasmons, respectively. Surprisingly, high spatial confinement and quality factor, also insensitive to n, can be simultaneously achieved in these terahertz DIPs. Their findings pave the way for developing topological plasmonic devices for stable terahertz applications.

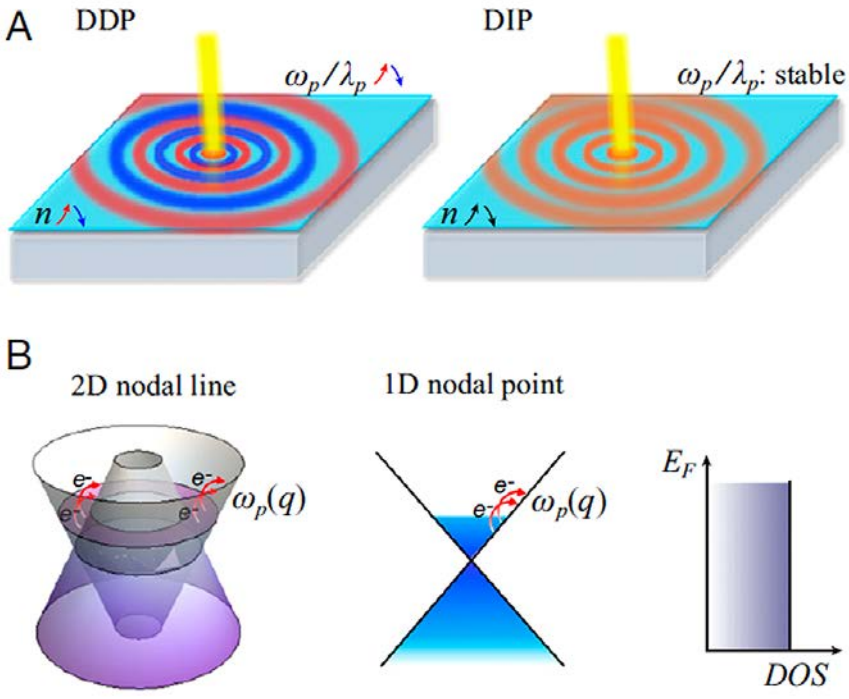


Fig. 1. (a) Comparison between conventional (left panel) and unconventional (right panel) plasmonic excitations. (b) Quantum material systems for the realization of unconventional plasmons.

非常规等离激元的普适理论和应用

(黄兵课题组)

为了将最先进的太赫兹技术有效地集成到紧凑型器件中，高度受限的太赫兹等离激元正受到广泛关注，处于基础研究和应用研究的最前沿。与金属中可见光频率范围的等离激元相比，太赫兹等离激元（通常存在于轻掺杂半导体或石墨烯中）对载流子密度（n）非常敏感，虽然易于调控，但是会导致不稳定或不精确的太赫兹光谱。最近，黄兵课题组首次通过推导一种简化但通用的等离激元频率表达形式，进而揭示了在不同维度的所有量子态中产生不寻常的等离激元（DIP）的统一机制。值得注意的是，课题组成员预测在二维节点线和一维节点系统中可以激发此类太赫兹范围的DIPs，这一点通过他们对几乎所有具有不同晶格对称性的拓扑半金属的第一性原理计算得到了证实。此外，DIPs中费米速度和简并因子依赖性的特性还可分别用于设计用于宽带太赫兹光谱和量子化太赫兹等离激元的拓扑超晶格和多壁碳纳米管超材料。令人惊讶的是，在这些系统中，也可以实现对n不敏感的高空间限制和质量因子。这些发现为开发用于稳定太赫兹应用的拓扑等离子体器件铺平了道路。

◀ 图 1　传统和非传统等离激发的表现形式及其在量子材料系统中的实现。

References:

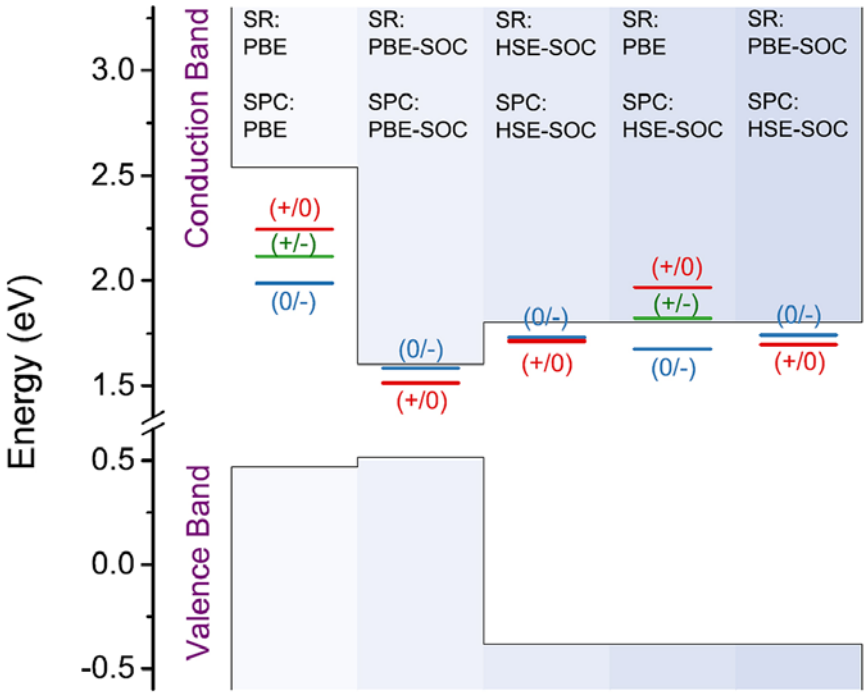
[1] J. F. Wang, X. L. Sui, W. H. Duan, F. Liu, and B. Huang*, *PNAS* 118, 2023029118 (2021).

POINT DEFECT PHYSICS IN LEAD HALIDE PEROVSKITES

(By Jun Kang)

In practical density-functional-theory-based simulations of defects in lead halide perovskites (LHPs), it is often assumed that spin-orbit coupling (SOC) and self-interaction corrections (SIC) mostly affect the electronic structure, whereas their effects on the structural properties are minor. Therefore, SOC and SIC are usually excluded during structural relaxation or molecular dynamics simulations. With such an assumption, previous studies predicted several unusual features of Br vacancies (VBr) in CsPbBr3, including the formation of a Pb dimer, negative-U character, and highly dynamic defect level. In this work, it is shown that SOC and SIC can play important roles in determining the equilibrium geometry and potential energy surface of VBr in CsPbBr3. Including SOC and SIC for structural relaxation results in a normal shallow level feature of VBr, instead of the negative-U character, and the Pb dimer becomes unstable in this case. Moreover, the highly dynamic defect level of VBr is absent when SOC is included for molecular dynamic trajectory generation. The contrasting results compared to previous studies are understood by the sensitive dependence of the occupation of the VBr-associated states on the band edge positions of CsPbBr3, which is greatly affected by the strong SOC and SIC. These results thus highlight the importance of the correct prediction of the band edge positions for accurate modeling of defects in LHPs. In addition, in an invited review by Appl. Phys. Rev., we summarize recent progress, made with the help of theoretical modeling, on atomic-scale understanding about intrinsic point defects and related processes in LHPs, including the fundamental properties of intrinsic point defects in LHPs, their impacts on structural properties and carriers of LHPs, and advanced strategies to engineer the defects in LHPs. Suggestions were provided for accurate modelling of defects in LHPs in the future.

Fig. 1. Calculated charge transition levels for VBr in CsPbBr3 using different schemes for structural relaxation and single-point calculation.



铅卤钙钛矿中的点缺陷物理

(康俊*)

在铅卤钙钛矿缺陷计算中，往往假设自旋轨道耦合（SOC）以及自能修正（SIC）效应对缺陷的晶格结构影响很小，因而长期被忽略。课题组的研究表明，对卤素空位而言，SOC和SIC会强烈影响带边位置，从而改变缺陷态的占据情况，这不仅仅引起能带结构的变化，也会改变缺陷的晶格结构。因此，此前的假设对这类缺陷不再适用，缺陷结构优化的过程需要采用修正SIC的杂化泛函，并考虑SOC。这些结果揭示了合理预测带边位置对于确定缺陷结构的重要影响。基于课题组在钙钛矿缺陷方面的系列研究基础，受 Appl. Phys. Rev. 邀请撰写钙钛矿点缺陷计算进展综述。综述系统回顾了钙钛矿本征点缺陷的基本物性，缺陷对结构和载流子的影响，已经调控缺陷特性的先进手段，并针对如何更加准确地模拟钙钛矿缺陷性质提出建议。

◀ 图 1　利用不同计算方法得到的CsPbBr3中Br空位缺陷电荷转换能级对比。

References:

[1] J. Kang*, *Phys. Rev. Mater.* 4, 085405 (2020).

[2] J. Kang*, J. Li, and S.-H. Wei, *Appl. Phys. Rev.* 8, 031302 (2021).

ACHIEVING ADJUSTABLE ELASTICITY WITH MECHANICAL METAMATERIALS

(By X. Shen, C. Fang, Z. Jin, H. Tong, S. Tang, H. Shen, N. Xu, J. H. Y. Lo*, **X. L. Xu***, and L. Xu*)

Mechanical systems with broadly adjustable elasticity are highly desired for various engineering and industrial applications, but are difficult to find in nature. Over the years people have strived for mechanical metamaterials with designed structures that respond flexibly to the external environment. Such materials have mostly been achieved by regular combination of identical units. However, disordered jamming structure, which are physically well defined and allow rigorous mathematical analysis, were recently discovered as another promising approach [1].

In a recent collaboration between the theoretical group led by Prof. Xinliang Xu at Beijing Computational Science Research Center and Prof. Lei Xu's experimental group at the Chinese University of Hong Kong, a topology-correlated transition between affine and non-affine regimes in elasticity is discovered, in both two- and three-dimensional packing-derived networks. Based on this transition, a continuous tunability in between solid-like affine response and liquid-like non-affine response can be achieved within a single system, which is then numerically designed and experimentally realized. In specific, the system exhibits a broadly tunable Poisson's ratio from positive to negative values, and tunable material strength with fixed Poisson's ratio (figure 1). This study reveals a fundamental connection between elasticity and network topology, and demonstrates its practical potential for designing mechanical systems and metamaterials [2].

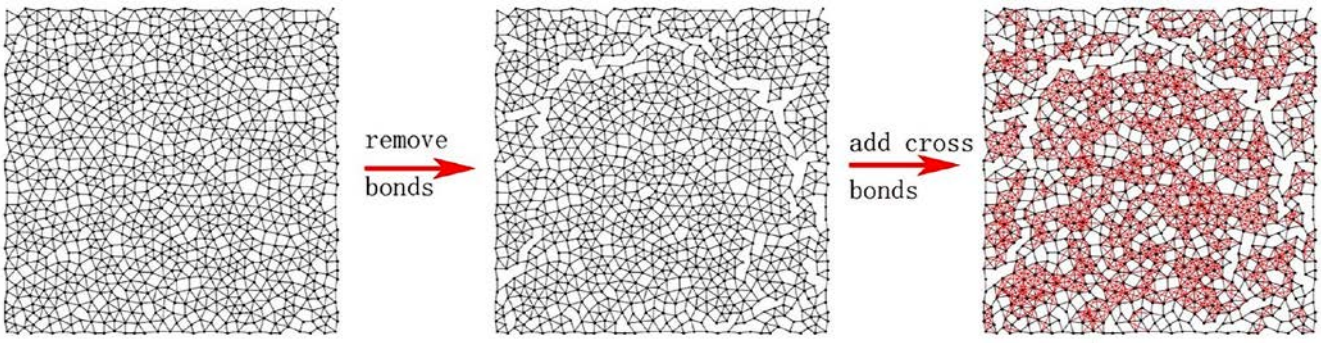


Fig. 1. By removing the right bonds we can tune system shear modulus (G) and bulk modulus (K) independently; by adding cross bonds in the complete triangulated areas, we can simultaneously raise both G and K with the ratio G/K fixed.

基于超构材料的弹性性质可调器件

（**沈翔瀛**，房臣超，Zhipeng Jin，童华，Shixiang Tang，Hongchuan Shen，徐宁，Jack Hau Yung Lo，**徐辛亮***，徐磊*）

弹性性质大范围可调的力学器件在工业生产生活中有很强的实用价值，但是在自然界中极为罕见。多年以来，人们一直希望通过超构材料结构的设计，实现在弹性性质方面能灵活反馈外力的功能器件。之前的研究主要集中于基于晶体结构的超构材料，对非晶结构研究的很少。通过最近一段时间的一系列严格数学分析，发现无序结构在设计超构材料结构方面也很有前途[1]。

最近，北京计算科学研究中心由徐辛亮教授领导的理论小组和香港中文大学徐磊教授领导的实验小组通力合作，在二维和三维力学网络系统中都发现了与系统拓扑性质相关的仿射-非仿射相变。基于这一相变，这些研究人员通过数值模拟和实验实现了一个力学弹性性质高度可调（从像固体一样的仿射式性质到像液体一样的非仿射式性质）的单一器件。具体来说，该器件既展示出从正到负高度可调的泊松比，又可以在保持泊松比不变的情况下增强整体的硬度（图一）。总的来说，这一研究一方面从基础的角度揭示了体系弹性性质和组份结构拓扑性质之间的关联，另一方面在设计基于超构材料的力学器件方面也展示了很强的使用价值。研究成果在领域内得到了广泛认可，最终在《自然 · 材料》杂志成文发表[2]。

◀ 图 1　在力学网络系统中，通过去除对剪切模量（G）或者体积模量（K）影响较大的链接，可以达到独立调控系统G和K的目的；同时，通过在完全三角化的区域添加交叉链接，可以同时增强G和K，而且保持G和K之比不变。

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[1] J. W. Rocks, N. Pashine, I. Bischofberger, C. P. Goodrich, A. J. Liu, and S. R. Nagel, Proc. Natl. Acad. Sci. USA **114**, 2520-2525 (2017).

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MODELING HYDRODYNAMIC INTERACTIONS IN ACTIVE FLUIDS

(By **Bokai Zhang**, P. Leishangthem, **Y. Ding***, and **X. L. Xu***)

Active suspensions of microswimmers demonstrate novel emergent behaviors (self-organization, active turbulence, etc.) on macroscopic length scales [1]. For such systems with, minimally, thousands of microswimmers, brute force approaches (e.g., boundary element method, or the method of Stokeslets) of the hydrodynamic interactions are just infeasible in the foreseeable future. In the meantime, existing reduced models are not satisfactory in describing the hydrodynamic interactions between microswimmers in close proximity with even qualitatively erroneous predictions, indicating a pressing need for an adequate model.

Theorists at Beijing Computational Science Research Center, led by Prof. Yang Ding from Mechanics Division, and Prof. Xinliang Xu from Complex Systems Division, recently proposed an effective model that solved this long-standing problem by capturing the essence of the hydrodynamic interactions through the resistance tensor. In a critical test case that studies the scattering angle of the pair dynamics between one E. coli bacterium and one passive sphere, it is proved that the near field hydrodynamic interaction can make a qualitative difference: Calculations based on the proposed model reveal a region in parameter space where the *E. coli* bacterium is trapped by the passive sphere, a phenomenon that is regularly observed in experiments but cannot be explained by any previous model (figure 1). Beyond its physical effectiveness, it is demonstrated that the model allows efficient simulation of active fluids with tens of thousands of microswimmers, sufficiently large for investigations of many emergent behaviors [2].

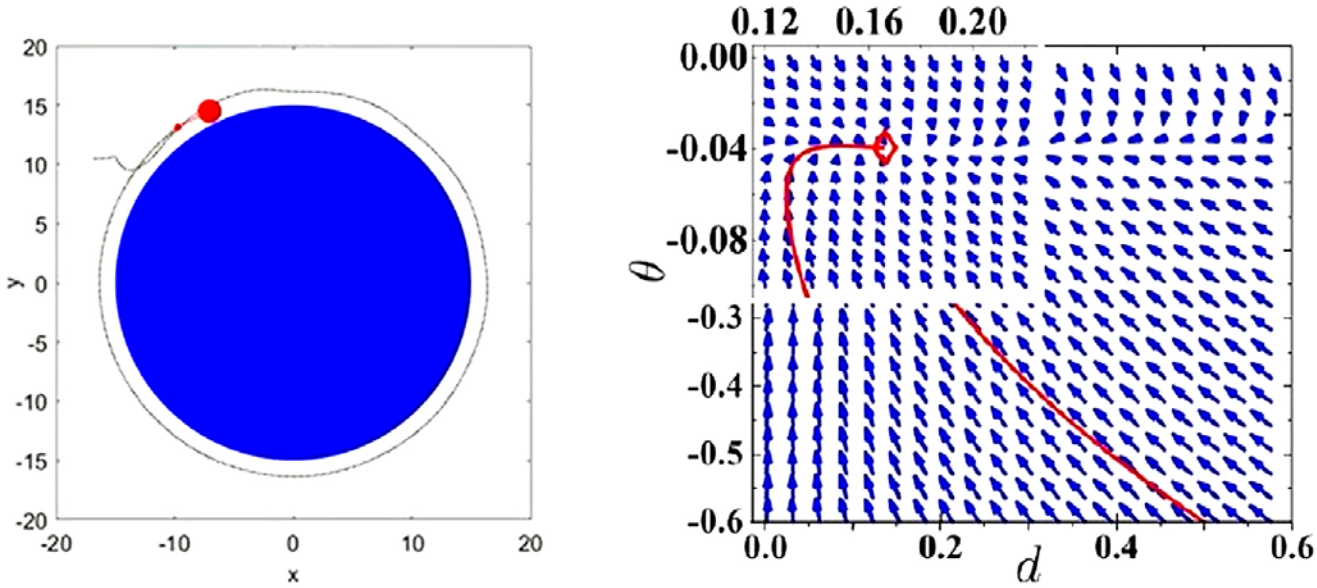

Fig. 1. The E. coli bacterium can be entrapped by the passive sphere with an orbital motion in real space (figure on the left), which can be related to a stable fixed point in the two-dimensional phase plane defined by the surface distance d, and incoming angle θ (figure on the right).

活性液体流体相互作用模型

（张博凯，Premkumar Leishangthem，丁阳*，徐辛亮*）

微生物溶液能在宏观尺度上展示很多新奇的涌现行为（自组织，活性湍流，等等）[1]。对于这样动辄成千上万个微生物个体的系统，对其中的流体相互作用进行暴力求解（如边界元方法，斯托克斯流等等）在可预见的将来都是力有不逮的。与此同时，现有的简化模型又不能很好的描述靠的很近的微生物之间的流体相互作用，甚至会出现定性性质方面的错误。要更好的了解这样的系统，急需一个既准确有高效的模型。

最近，北京计算科学研究中心由力学部丁阳教授和复杂体系研究部徐辛亮教授领导的两个小组通力合作，提出了一个有效模型，解决了这个困扰了人们多年的问题。在这个有效模型中，通过使用阻尼矩阵，有效地描述了活性体系中的流体相互作用。在一个重要的测试项目中，这个有效模型被用来研究一个大肠杆菌和一个标记球的两体散射动力学，并证明了近邻之间的流体相互作用对于动力学有着举足轻重的作用：通过有效模型的计算，发现大肠杆菌可以像在实验中被多次观测到的那样被标记球捕获，进行轨道运动（图一），而之前的模型都无法做到这样的结果。除了能准确地抓住流体相互作用的精髓，这个有效模型还可以很轻松的实现对成千上万个微生物个体的计算模拟，满足人们研究活性液体中多种涌现行为的需求。研究成果在领域内得到了广泛认可，最终在《美国科学院院报》杂志成文发表[2]。

◀ 图 1　大肠杆菌可以被标记球捕获，进行轨道运动（左图）。这一行为在像空间对应一个稳定的不动点（右图）。

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ANALYSIS OF ADAPTIVE BDF2 SCHEME FOR DIFFUSION EQUATIONS

(By Hong-lin Liao, Zhimin Zhang*)

For linear and nonlinear parabolic problems, the stability and convergence of multi-step approaches with unequal time-steps would be challenging because they involve multiple degrees (including the current step size τ_n, the previous step size τ_{n-1} and so on) of freedom. Due to its strong stability, the variable two-step backward differentiation formula (BDF2) is practically valuable for stiff or differential-algebraic problems. But **the stability and convergence theory remains incomplete so far**, even for the simplest linear heat equation $\partial_t u = \Delta u + \kappa u + f$.

There are many existing stability results. The variable-step BDF2 method for nonlinear ODE problems was shown by Grigorieff (Numer.Math.,1983,42:359-377) to be zero-stable if and only if the adjacent time-step ratios $0 < r_k := {}^{\tau_k}/_{\tau_{k-1}} < 1 + \sqrt{2} \approx 2.414$. If $0 < r_k < \frac{2+\sqrt{13}}{3} \approx 1.868$, Becker (BIT,1998,38:644-662) established the well-known $\boldsymbol{L}^2$ norm estimate,

$$\|u^n\| \le C_r e^{C_r \Gamma_n} \left(\|u^0\| + \sum_{i=1}^{n} \tau_i \|f^i\| \right)$$

where the quantity $\Gamma_n = \sum_{k=2}^{n-2} max\{0, r_k - r_{k+2}\}$ **may take the value zero, bounded or unbounded** at vanishing step sizes by choosing certain step-ratio sequences $\{r_k\}$. Emmrich (J. Appl. Math. & Computing,2005,19:33-55) improved slightly the step-ratio restriction to $0 < r_k < 1.91$, but continued to retain the undesirable prefactor $e^{C_r \Gamma_n}$. Chen et al (SIAM J. Numer. Anal., 2019, 57:495-525) replaced the undesirable prefactor $e^{C_r \Gamma_n}$ with $e^{C_r t_n}$ under the step-ratios condition $0 < r_k < 1.53$. Their new estimate avoids the worst case of Γ_n being unbounded, but may lose some other approximately ideal situations with $\Gamma_n = 0$.

Our work starts from **a new viewpoint**, that is, views the BDF2 formula as a discrete convolution summation,

$$D_2 v^n = \sum_{k=1}^{n} b_{n-k}^{(n)} (v^k - v^{k-1})$$

where the discrete convolution kernels $b_{n-k}^{(n)}$ are defined by $b_0^{(1)} = 1/\tau_1$, and when $n \ge 2$, $b_0^{(n)} = \frac{1+2r_n}{\tau_n(1+r_n)}$, $b_1^{(n)} = \frac{r_n^2}{\tau_n(1+r_n)}$ and $b_j^{(n)} = 0$ for $2 \le j \le n-1$. **A new discrete tool**, namely, discrete orthogonal convolution (DOC) kernels $\theta_{n-j}^{(n)}$, was introduced at the first time by a recursive procedure $\theta_0^{(n)} = \frac{1}{b_0^{(n)}}$ and $\theta_{n-j}^{(n)} = \frac{1}{b_0^{(j)}} \sum_{k=j+1}^{n} \theta_{n-k}^{(n)} b_{k-j}^{(k)}$ for $1 \le j \le n-1$.

The DOC kernels $\theta_{n-j}^{(n)}$ satisfy the orthogonal identity with the Kronecker delta symbol δ_{nk}, $\sum_{j=k}^{n} \theta_{n-j}^{(n)} b_{j-k}^{(j)} = \delta_{nk}$ for $1 \le k \le n$. We prove that the DOC kernels are positive, decaying and positive semi-definite if the adjacent time-step ratios $0 < r_k < 3.651$. Consider the following adaptive BDF2 time-stepping scheme $D_2 u^k = \varepsilon \Delta u^k + \kappa(x)\, u^k + f^k$ for $1 \le k \le N$. We adopt a new technical path by transforming this local formulation at time t_k into a discrete convolution summation containing all previous information, $u^k - u^{k-1} = \sum_{j=1}^{k} \theta_{k-j}^{(k)} \left[\varepsilon \Delta u^j + \kappa(x)\, u^j \right] + \sum_{j=1}^{k} \theta_{k-j}^{(k)} f^j$ for $1 \le k \le N$. By this nonlocal formulation, we obtain some concise $\boldsymbol{L}^2$ norm stability and convergence estimates, so that they look similar to those of the simplest BDF1 scheme. They naturally remove the undesirable prefactor $e^{C_r \Gamma_n}$ or $e^{C_r t_n}$ if the reaction coefficient is non-positive.

At the first time, we prove theoretically that **the widespread variable-step BDF2 scheme is mesh-robustly stable and convergent in the $\boldsymbol{L}^2$ norm**. It seems that the proposed DOC kernels and the present technical framework open new doors to investigate the variable-step or adaptive time-stepping approaches theoretically in time integrations of partial differential equations.

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扩散方程变步长BDF2格式的数值分析

(廖洪林，张智民*)

对于线性和非线性抛物方程，变步长多步方法的稳定性和收敛性分析往往很困难，这主要是因为它们涉及多个自由变量（包括当前时间步长τ_n，前一个时间步长τ_{n-1}，等等）。近四十年来，因其良好的计算稳定性以及对高频波的耗散性，变步长BDF2格式在刚性系统以及微分-代数系统的时间积分中有非常广泛的实际应用。相比之下，即便对于最简单的线性热传导方程，如 $\partial_t u = \Delta u + \kappa u + f$，相应的稳定性和收敛性理论至今仍是非常不完整的, 现有的一些结论也存在关键性缺陷.

早在1983年，Grigorieff (Numer.Math.,1983,42:359-377)证明变步长BDF2格式对满足Lip条件的非线性常微分方程是零稳定的，当且仅当相邻时间步长比 $r_k := \tau_k/\tau_{k-1}$ 满足 $0 < r_k < 1 + \sqrt{2} \approx 2.414$. 对于线性热传导方程，Becker (BIT,1998,38:644-662)在步长比条件 $0 < r_k < \frac{2+\sqrt{13}}{3} \approx 1.868$ 下建立例如如下经典 L^2 模稳定性估计

$$\|u^n\| \le C_r e^{C_r \Gamma_n}\left(\|u^0\| + \sum_{i=1}^{n} \tau_i \|f^i\|\right)$$

这个离散估计式与连续解的 L^2 模稳定性估计相去甚远，其最大缺陷是引入一个与步长比相关的量 $\Gamma_n = \sum_{k=2}^{n-2} max\{0, r_k - r_{k+2}\}$. 我们可以选择特定的步长比序列 $\{r_k\}$, 使得 Γ_n 取为0，有限值或无穷大，也就是说，这个 Γ_n 是一个无界量. Emmrich (J. Appl. Math. & Computing,2005,19:33-55) 将Becker给出的步长比条件改进为 $0 < r_k < 1.91$, 但上述估计式中的最大缺陷，即前置因子 $e^{C_r \Gamma_n}$，被保留了下来。最近，Chen 等学者 (SIAM J. Numer. Anal., 2019, 57:495-525) 通过一个改进的离散Gronwall不等式，将稳定性估计中的前置因子 $e^{C_r \Gamma_n}$ 替换为 $e^{C_r t_n}$（在有限时间T内是有界的），但相应的估计似乎要求一个更严格步长比限制，即 $0 < r_k < 1.53$. 显然，Chen 等学者所给的新估计剔除了前置因子中的无界量，但与连续解的 L^2 模稳定性估计还是有差距的，或者说，新估计也漏掉了某些理想状态，如 $\Gamma_n = 0$ 的情形.

我们的工作从一个新的视角出发，即首先把变步长BDF2格式看成一个离散卷积和，$D_2 v^n = \sum_{k=1}^{n} b_{n-k}^{(n)} (v^k - v^{k-1})$. 其中，相应的离散卷积核 $b_{n-k}^{(n)}$ 定义为 $b_0^{(1)} = 1/\tau_1$, 而当时间层指标 $n \ge 2$ 时, $b_0^{(n)} = \frac{1+2r_n}{\tau_n(1+r_n)}$, $b_1^{(n)} = \frac{r_n^2}{\tau_n(1+r_n)}$ 以及 $b_j^{(n)} = 0$, $2 \le j \le n-1$.写成上述离散卷积和形式的主要目的在于引入一个新的离散工具，即所谓的DOC (discrete orthogonal convolution) 卷积核 $\theta_{n-j}^{(n)}$. 它可以由以下递推式来定义，$\theta_0^{(n)} = \frac{1}{b_0^{(n)}}$ and $\theta_{n-j}^{(n)} = \frac{1}{b_0^{(j)}} \sum_{k=j+1}^{n} \theta_{n-k}^{(n)} b_{k-j}^{(k)}$ for $1 \le j \le n-1$. 显然，DOC卷积核 $\theta_{n-j}^{(n)}$ 满足一个离散正交恒等式 (这里，δ_{nk} 是Kronecker符号) $\sum_{j=k}^{n} \theta_{n-j}^{(n)} b_{j-k}^{(j)} = \delta_{nk}$ for $1 \le k \le n$. 可以证明，如果步长比满足 $0 < r_k < 3.651$，上述DOC卷积核 $\theta_{n-j}^{(n)}$ 是正的、衰减，也是正半定的（在二次型意义下）. 为简单起见，仅考虑一个线性扩散方程的变步长BDF2时间离散格式 $D_2 u^k = \varepsilon \Delta u^k + \kappa(x)\, u^k + f^k, 1 \le k \le N$. 借助于DOC核 $\theta_{n-j}^{(n)}$ 以及相应的离散正交恒等式，我们可以把上述建立在时间层 t_k 上的 BDF2时间离散格式转化为一个包含所有历史信息、以DOC核 $\theta_{n-j}^{(n)}$ 为权重的离散卷积和形式, $u^k - u^{k-1} = \sum_{j=1}^{k} \theta_{k-j}^{(k)} \left[\varepsilon \Delta u^j + \kappa(x)\, u^j\right] + \sum_{j=1}^{k} \theta_{k-j}^{(k)} f^j$, $1 \le k \le N$. 新的离散能量估计都是从这个非局部形式出发的。我们由此给出了一些非常简洁的 L^2 模稳定性与收敛性估计, 它们很好地模拟了连续解的 L^2 模估计，以致于和最简单BDF1格式的相关结果相差无几。显然，从数值分析的角度，这些理论结果本质上克服了长期以来变步长BDF2格式的相关理论缺陷，也更新了人们对该方法的理解.

应该说，这是第一次在理论上证明：变步长BDF2格式的 L^2 模稳定性和收敛性对步长变化具有很强的鲁棒性。在一定意义上，本文所采用的DOC技术也为更一般的变步长或自适应时间积分方法的理论探讨开启了一个新窗口。

ENERGY-PRODUCTION-RATE PRESERVING NUMERICAL APPROXIMATIONS TO NETWORK GENERATING PARTIAL DIFFERENTIAL EQUATIONS

(By **Qi Hong**, Jia Zhao and **Qi Wang**)

We propose a network generating partial differential equation (PDE) system in the form of gradient flows, which reduces to the thermodynamically consistent, dissipative network generating PDE model at a singular limit. Using the energy quadratization method, we reformulate the gradient flow system into an equivalent form with a quadratic energy density by introducing auxiliary variables. We then devise a series of fully discrete, finite difference, linear, second order, and energy-production rate preserving numerical algorithms to solve the quadratized PDE system subject to various compatible boundary conditions. We show that the numerical schemes are energy-production-rate preserving for any time steps.

Numerical convergence tests are given to validate the accuracy of the fully discrete schemes. Several 2D numerical examples are shown to demonstrate the capability of the schemes in predicting network generating phenomena with the gradient flow PDE system, especially, the dissipative network generating PDE model. This provides a systematic approach to develop energy-production-rate preserving numerical algorithms for PDE models describing coupled diffusion phenomena.

Biological transport networks have a vitally important role in plant growth, nutrient, and materials transport in living organisms. They have drawn increasing research interests due to their ubiquitous existence in living organisms and rich phenomena exhibited in nature, two examples of which are the leaf venation in plants and blood flow network in animals. Recently, Cai and Hu proposed a discrete model which can be reformulated into a system of ordinary differential equations (ODEs) to study network dynamics [1]. A generalized PDE version is henceforth proposed to model network generating phenomena [1, 2]. This PDE model consists of a spatial-temporal PDE system for a vector conductance variable and an elliptic constraint equation in space for a pressure-like variable. This model has been shown to have the ability to form a network with a given source and is thermodynamically consistent with a negative definite energy production rate functional. Therefore, it is dissipative. We henceforth call it the dissipative network generating PDE model in this paper. In a series of studies, the thermodynamic structure and solution behavior of the model have been further analyzed [2,3,4,5].

We briefly recall the dissipative, network generating PDE model proposed in [1,2,4,5]. Consider a bounded domain Ω with a smooth boundary $\partial\Omega$ and a time-independent source term $S(x)$. Here we use p to represent the scalar pressure of the fluid transported within the network and $\mathbf{m}$ for the vector-valued conductance. The dissipative network generating PDE system consists of two equations

$$-\nabla\cdot\left((r\mathbf{I}+\mathbf{mm})\nabla\mathbf{p}\right)=\mathbf{S},$$

$$\mathbf{m}_t-\mathbf{K}\Delta\mathbf{m}-\mathbf{a}^2(\mathbf{m}\cdot\nabla\mathbf{p})\nabla\mathbf{p}+\boldsymbol{\alpha}\,|\,\mathbf{m}\,|^{2(\gamma-1)}\,\mathbf{m}=\mathbf{0},$$

subject to homogeneous Dirichlet boundary conditions for $\mathbf{m}$ and p at $\partial\Omega$:

$$\mathbf{m}(t,\mathbf{x})=0,\quad p(t,\mathbf{x})=0,\quad \forall\,\mathbf{x}\in\partial\Omega,\quad t\geq 0.$$

Here the model parameters are diffusivity $K\geq 0$, $r,\gamma,\alpha>0$, and activation parameter $a>0$. One deduces from the model the following energy production rate equation

$$\frac{\mathrm{dE}}{\mathrm{d}t}=-\int_\Omega\|\partial_t\mathbf{m}\|\,\mathrm{d}x,$$

where the energy functional is defined by

$$\mathrm{E}=\frac{1}{2}\int_\Omega\left(K\,|\,\nabla\mathbf{m}\,|^2+\frac{\alpha}{\gamma}\,|\,\mathbf{m}\,|^{2\gamma}+a^2\,|\,\mathbf{m}\cdot\nabla p\,|^2+a^2r\,|\,\nabla p\,|^2\right)\mathrm{dx}.$$

Recognizing that the dissipative network-generating PDE system can be viewed as a singular limit of a gradient flow system by introducing a relaxation dynamics to the equation of pressure like variable p, we extend the network generating PDE

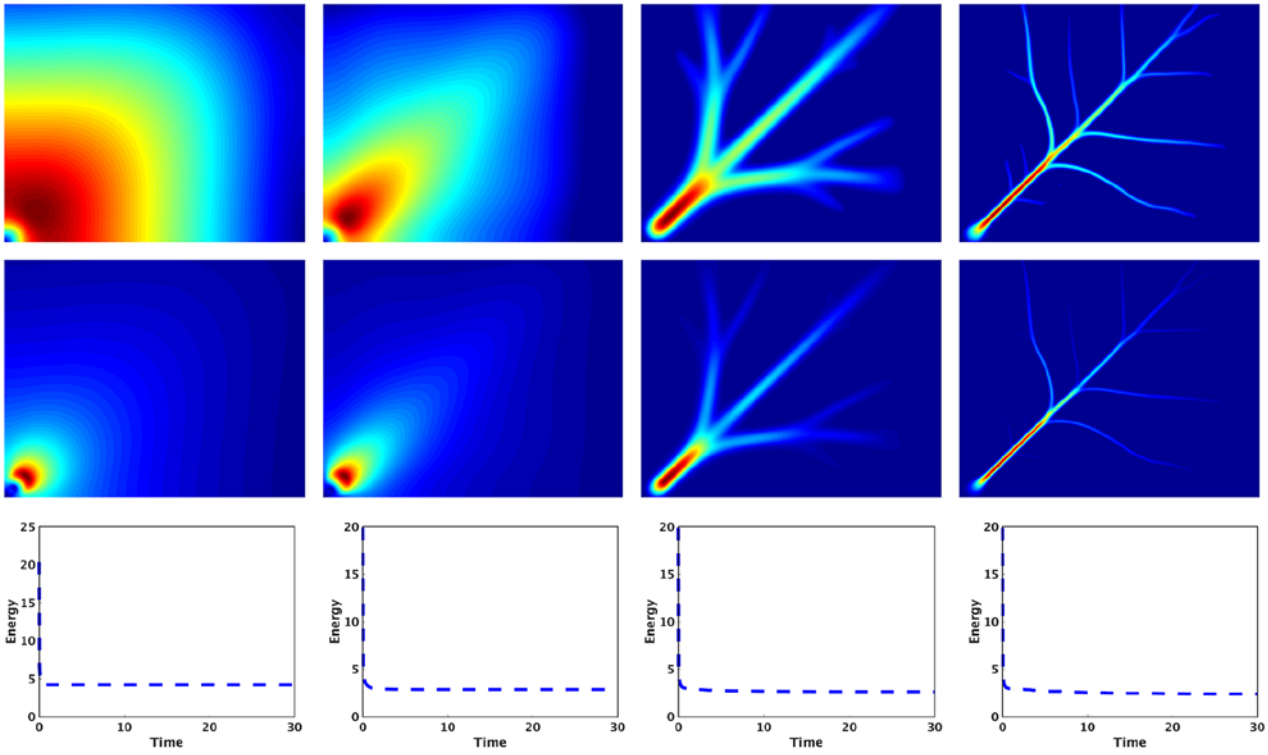

Fig. 1. Effect of diffusion coefficient K on the network formation. The conduction vector m (top), fluid velocity v (middle) in the norm scale and the energy with $K=0.5^2$, 0.1^2, 0.02^2, 0.005^2 (from first colume to last column), are shown respectively. Here we observed diffusion coefficient K controls the spatial scale/resolution of network structure, and smaller diffusion coefficient will enhance the sharper network structure formation.

model to a more general network generating gradient flow system. We apply the energy quadratization strategy in time to develop linear, energy production rate preserving schemes [6] that respect the energy dissipation law at the fully discrete level for the gradient flow system.

Fig 1 shows a couple numerical results where a time-independent source leads to the formation of a branched network structures.

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网络生长偏微分方程的保能量耗散率的数值算法

（洪旗，赵佳，王奇）

本文提出了一个梯度流形式的网络生长偏微分方程 (PDE) 系统，该系统在奇异极限下退化为热力学一致的耗散网络增长模型。利用能量二次化方法，通过引入辅助变量，将梯度流系统转换成具有二次能量密度的等价形式。然后，我们设计了一系列的全离散的、有限差分的、线性的、二阶的、保持能量耗散率的数值算法，求解在各种相容边界条件下的二次化的偏微分方程系统。我们证明了该数值格式对于任何时间步长都能保持能量耗散率。数值收敛测试验证了该格式的精度。 一些2维数值实验验证了全离散格式能够预测该梯度流形式的PDE具有网络生长现象，特别是对耗散网络生成偏微分方程模型的预测能力。这为开发描述耦合扩散现象的偏微分方程模型的保能量耗散率的数值算法提供了一种系统化的方法。

生物网络增长模型在生物体内的生长、营养和物质运输中起着至关重要的作用。于它们在生物体内的普遍存在和在自然界中表现出的丰富的现象，引起了人们越来越多的研究兴趣。植物的叶脉和动物的血流网络就是其中的两个突出的例子。前几年，蔡申瓯和胡丹提出了一种可以表述为常微分方程组 (ODEs) 的离散模型来研究网络动力学[1]。文献[1, 2]提出了一种广义的PDE模型来模拟网络增长现象。该模型由矢量电导变量的时空偏微分方程和压力类变量的空间椭圆约束方程组成。该模型已被证明具有与给定源形成网络的能力，并且在热力学上符合能量耗散原理。所以，本文称之为耗散网络生成偏微分方程模型。我们在一系列的研究中，进一步分析了该模型的热力学结构和解的行为。

我们简要回顾文献[1,2,4,5]中提出的具有耗散性质的网络生长模型。考虑具有光滑边界的有界区域和不依赖时间的源项 $S(x)$，这里使用标量p 表示在网络内传输的“流体”压力，和 $\mathbf{m}$ 表示向量电导值. 耗散网络生长PDE系统由下面两个方程组成:

$$-\nabla\cdot\left((r\mathbf{I}+\mathbf{mm})\nabla\mathbf{p}\right)=\mathbf{S},$$
$$\mathbf{m}_t-\mathbf{K}\Delta\mathbf{m}-\mathbf{a}^2(\mathbf{m}\cdot\nabla\mathbf{p})\nabla\mathbf{p}+\boldsymbol{\alpha}\,|\,\mathbf{m}\,|^{2(\gamma-1)}\,\mathbf{m}=\mathbf{0},$$

其中，p 和 $\mathbf{m}$ 在边界 $\partial\Omega$ 上满足齐次Dirichlet边界条件:

$$\mathbf{m}(t,\mathbf{x})=0,\quad p(t,\mathbf{x})=0,\quad \forall\,\mathbf{x}\in\partial\Omega,\quad t\geq 0.$$

这里的模型参数是扩散系统 $K\geq 0$, $r,\gamma,\alpha>0$, 激活参数 $a>0$. 该模型有如下的能量耗散率方程:

$$\frac{\mathrm{dE}}{\mathrm{d}t}=-\int_\Omega\|\partial_t\mathbf{m}\|\,\mathrm{d}x,$$

其中，能量泛函 定义为:

$$\mathrm{E}=\frac{1}{2}\int_\Omega\left(K\,|\,\nabla\mathbf{m}\,|^2+\frac{\alpha}{\gamma}\,|\,\mathbf{m}\,|^{2\gamma}+a^2\,|\,\mathbf{m}\cdot\nabla p\,|^2+a^2r\,|\,\nabla p\,|^2\right)\mathrm{d}x.$$

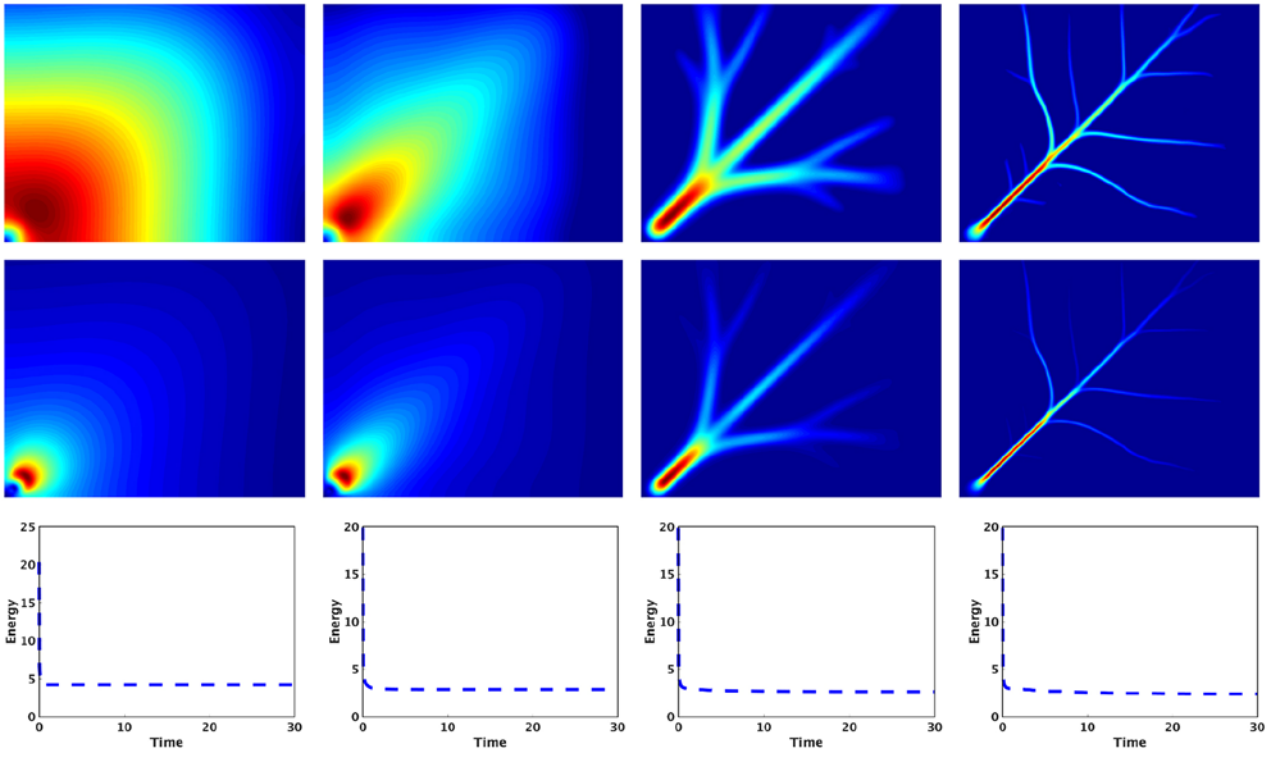

图 1　扩散系数 K 对网络形成的影响. 在范数意义下，电导向量 m (top), 流体速度 v (middle) 和能量，其中 K= 0.5^2, 0.1^2, 0.02^2, 0.005^2 (从第一列到最后一列). 从图中可以清晰地观察到扩散系数 K 影响网络的结构，较小的扩散系数增强了更尖锐的网络结构的形成.

注意到耗散性网络生长PDE系统可以被看作是梯度流系统的一个奇异极限，通过对类似压力变量 p 的方程引入松弛动力学，我们将网络生成PDE模型扩展到更普遍的网络增长梯度流系统. 我们在时间上应用能量二次化策略，设计线性的、保能量产生率的全离散数值格式 [6] 求解这个梯度流系统. 图1展示了我们热力学一致、二阶数值算法的计算结果。由源项生成的网络清晰可见。

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CONVERGENCE OF A SECOND-ORDER ENERGY-DECAYING METHOD FOR THE VISCOUS ROTATING SHALLOW WATER EQUATION

(By Georgios Akrivis, Buyang Li, **Jilu Wang**)

The shallow water equations describe the evolution of an incompressible fluid in response to gravitational and rotational accelerations for small enough ratio between the vertical and the horizontal scales. They are typically used to describe vertically averaged flows in three-dimensional domains in terms of horizontal velocity and depth variation. Many efforts have been devoted to developing efficient numerical methods and analyzing stability and convergence of numerical solutions for the shallow water equation, e.g., the semi-implicit finite element methods (FEMs), the leap-frog FEMs, the explicit Runge-Kutta FEMs, the nonlinearly implicit characteristic method, and exponential time differencing methods. As far as we know, all existing error analyses of implicit and linearly implicit time-stepping methods for the viscous shallow water equation require the grid-ratio condition $\tau = O(h^2)$, which is natural for the hyperbolic shallow water equation but may not be necessary for the viscous model. Otherwise the semidiscretization in time (corresponding to the case $h \to 0$ in the full discretization) may not converge with optimal-order.

Recently, Georgios Akrivis (University of Ioannina), Buyang Li (The Hong Kong Polytechnic University), and Jilu Wang (CSRC) investigate an implicit energy-decaying modified Crank-Nicolson time-stepping method for the viscous rotating shallow water equation on the plane

$$\partial_t H = -\nabla \cdot (Hu) \tag{1}$$

$$\partial_t u = -\nabla\Big(\frac{1}{2}|u|^2 + g(H - H_b)\Big) - (\nabla \times u + f)\hat{k} \times u + \mathcal{G}(H,u) \tag{2}$$

where $H: \Omega \times [0,T] \to \mathbb{R}$ and $u = (u_1, u_2)^T: \Omega \times [0,T] \to \mathbb{R}^2$ denote the fluid thickness and velocity, respectively, and

$$\mathcal{G}(H,u) = \frac{\mu}{H}\nabla \cdot (H\nabla u) - c_f \frac{|u|u}{H}$$

consists of the viscous and friction forces, with $|u|$ denoting the magnitude of the velocity u.

The paper [1] proposes a second-order energy-decaying modified Crank-Nicolson method for the viscous problem (1)-(2) and establish optimal-order convergence of the semidiscretization method in the H^2 norm with respect to the time stepsize. This would provide a foundation for error analysis of fully discrete FEMs using the error splitting approach [2,3] without a grid-ratio condition. The analysis of H^2 convergence of the proposed nonlinearly implicit temporal semidiscretization for the hyperbolic-parabolic system (1)-(2) is different from all existing work using the error splitting approach, e.g., [2,3], which all concern only nonlinear parabolic equations and linearly semi-implicit schemes. The derivation of the error estimates in this paper is based on the boundedness of the numerical solutions in $H^2(\Omega)$ (uniformly with respect to the stepsize τ), proved by Schaefer's fixed-point theorem, combined with discrete $L^\infty(0,T;H^2(\Omega))$ and $L^2(0,T;H^3(\Omega))$ estimates of the Crank-Nicolson scheme. The energy of numerical solutions is presented in Fig. 1, which shows that the energy decays in time.

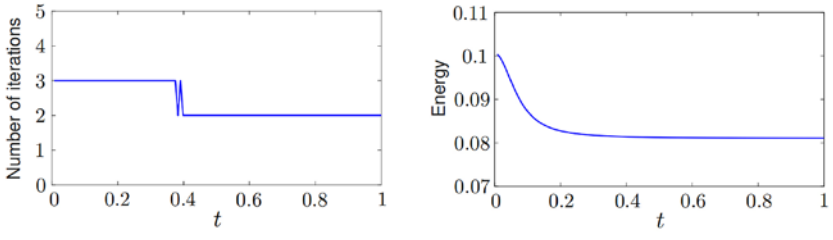

Fig. 1. Number of iterations and energy at each time level

图 1　每个时间层迭代的次数和能量

粘性旋转浅水波方程二阶能量递减方法的收敛性分析

(Georgios Akrivis，李步扬，王冀鲁)

浅水波方程描述了当垂直方向尺度远小于水平方向尺度时，不可压缩流体在重力和旋转加速度作用下的运动规律。该方程通常用于刻画三维区域中垂直平均流体水平速度和深度的变化规律。人们已经发展了很多有效的数值方法求解浅水波方程，并且分析了相应数值解的收敛性和稳定性。这些数值方法包括半隐有限元方法、蛙跳有限元方法、显式 Runge-Kutta 有限元方法、非线性隐式特征线法以及指数时间差分方法。据我们所知，目前现有关于粘性浅水波方程隐式及线性化隐式离散方法的误差分析都需要网格比条件 $\tau = O(h^2)$。该条件对于双曲型浅水波方程是自然的，但对于粘性模型可能不是必需的。否则，时间半离散格式（对应于全离散数值格式在 $h \to 0$ 时的情况）可能不会以最优收敛阶收敛。

最近，Georgios Akrivis (约阿尼纳大学)、李步扬（香港理工大学）、王冀鲁（北京计算科学研究中心）研究了平面上粘性旋转浅水波方程具有能量递减性质的隐式修正 Crank-Nicolson 时间离散方法:

$$\partial_t H = -\nabla \cdot (Hu) \tag{1}$$

$$\partial_t u = -\nabla\left(\frac{1}{2}|u|^2 + g(H - H_b)\right) - (\nabla \times u + f)\hat{k} \times u + \mathcal{G}(H,u) \tag{2}$$

这里，$H:\Omega \times [0,T] \to \mathbb{R}$ 和 $u = (u_1,u_2)^T:\Omega \times [0,T] \to \mathbb{R}^2$ 分别代表流体的深度和速度。

$$\mathcal{G}(H,u) = \frac{\mu}{H}\nabla \cdot (H\nabla u) - c_f \frac{|u|u}{H}$$

是跟粘性力和摩擦力有关的函数，其中 $|u|$ 代表速度的大小。

文章[1]对粘性浅水波方程(1)-(2)提出了一种具有能量递减性质的二阶修正 Crank-Nicolson 方法，并建立了时间半离散方法的 H^2 最优收敛性分析。该结果将为使用误差分裂技巧[2,3]分析全离散有限元方法提供理论基础。该文章中关于非线性隐式时间半离散格式的分析不同于现有使用误差分裂方法的工作，例如[2,3]。这些工作都是针对非线性抛物方程和线性化半隐格式。而文章[1]中误差估计的推导是基于数值解在 $H^2(\Omega)$ 范数下关于时间步长 τ 的一致有界性。该一致有界性是基于 Schaefer 不动点定理，并结合Crank-Nicolson方法离散 $L^\infty(0,T;H^2(\Omega))$ 和 $L^2(0,T;H^3(\Omega))$ 估计得到的。图1给出了数值解的能量变化规律，表明能量是随着时间递减的。

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FREQUENCY DOMAIN ANALYSIS OF FLUCTUATIONS OF MRNA AND PROTEIN COPY NUMBERS WITHIN A CELL LINEAGE: THEORY AND EXPERIMENTAL VALIDATION

(By **Chen Jia**#, Ramon Grima*)

Over the past two decades, significant progress has been made in the theory and experiments of single-cell gene expression dynamics. Classical gene expression models [1] have not considered various cell cycle features, and thus cannot describe the time-course data of single cell lineages. In a recent paper [2], Chen Jia from CSRC and Ramon Grima from the University of Edinburgh have developed a detailed model of stochastic gene expression dynamics with a high level of biological realism which includes transcription, translation, bursting, degradation, promoter switching, cell cycle duration variability, gene replication, gene dosage compensation, cell division, and size homeostasis. Moreover, for the first time, they have calculated in closed form the power spectrum of gene expression levels along a cell lineage and investigated stochastic oscillations of single-cell lineage measurements. The analytical expressions provide insights into how the regularity and noisiness of the oscillations in the gene product abundance across generations are related to the rate parameters associated with various subcellular processes at play. The theory also makes various predictions that are then verified by analysis of a publicly available single-cell gene expression dataset of Escherichia coli followed over 70 generations in three different growth conditions. Finally, they have shown how matching the experimental and theoretical power spectra enables a reliable inference of gene expression rate parameters.

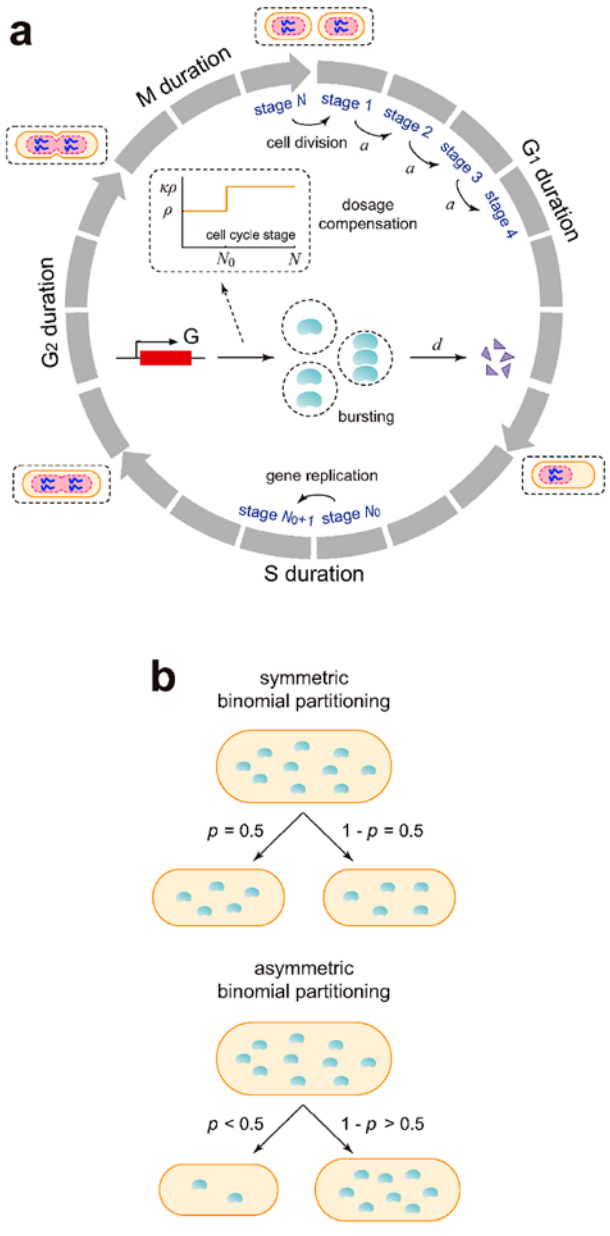

Fig. 1. A detailed gene expression model across the cell cycle. (a) Schematic illustrating the model describing N effective cell cycle stages, gene replication at stage *No*, bursty production of the gene product, degradation of the gene product, and gene dosage compensation induced by a change in the burst production rate upon replication from ρ to $\kappa\rho$ with $\kappa < 2$ (see inset graph). (b) At stage *N*, a mother cell divides into two daughters that are typically different in size (asymmetric division) with the larger daughter inheriting more molecules. Symmetric division is the special case where the daughters are equisized.

单细胞谱系基因表达拷贝数涨落的频域分析：理论与实验验证

(贾晨#，Ramon Grima*)

近二十年来，单细胞随机基因表达动力学的理论与实验取得了突破性进展。经典的基因表达模型[1]没有考虑各种细胞周期特征，因此无法描述单细胞谱系的时间序列测量。在一项最近的工作中[2]，北京计算科学研究中心的贾晨研究员与英国爱丁堡大学的Ramon Grima教授建立了单细胞谱系随机基因表达动力学的具有高度生物学实际的精细模型。该模型考虑了多种重要的生物学因素，包括转录、翻译、基因产物的爆发性、基因产物的降解、基因切换、细胞周期时间的变异性、基因复制、基因计量补偿、细胞分裂、尺寸动态平衡等。此外，该工作首次得到了单细胞谱系基因表达拷贝数功率谱的解析解，并研究了单细胞谱系测量由于细胞周期所诱导的随机振荡行为。功率谱的解析表达式可以帮助人们更深入地理解基因产物分子数随机振荡的规则性与噪声性是如何受到细胞内各种生化过程的速率参数的影响。该理论衍生出大量的生物学预测，他们进一步通过分析大肠杆菌的单细胞公共数据集对理论进行了实验验证，该数据集包括三个温度下大肠杆菌蛋白表达量的单细胞谱系数据，每个细胞谱系包含70个细胞周期。最后，通过对实验功率谱与理论功率谱进行匹配，他们对模型中所有的基因表达速率参数进行了可信的推断。

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◀ 图 1　单细胞谱系基因表达随机动力学的精细模型. (a) 模型的示意图。该模型描述了 N 个等效的细胞周期状态，基因产物的爆发性产生，基因产物的降解，基因复制，以及基因计量补偿。基因复制发生在第N0个细胞周期状态，基因计量补偿由爆发频率在基因复制时由 ρ 变为 $\kappa\rho$ 所诱导，其中 $\kappa < 2$（见内图）。(b) 在第 N 个细胞周期状态，母细胞分裂为两个子细胞，两个子细胞的体积通常是不同的，即非对称分裂。体积更大的子细胞继承了更多的基因产物分子。对称分裂对应于两个子细胞体积相同的特殊情形。

BLOW-UP OF ERROR ESTIMATES IN TIME-FRACTIONAL INITIAL-BOUNDARY VALUE PROBLEMS

(By Hu Chen and **Martin Stynes***)

Let $\alpha \in (0,1)$ be fixed. Consider the time-fractional initial-boundary value problem (IBVP) $D_t^\alpha u - p\Delta u + c(x)u = f(x,t)$ for $(x,t) \in Q := \Omega \times (0,T)$, where Ω is a bounded domain in $\mathbb{R}^d$ and $d \in \{1,2,3\}$, subject to the initial condition $u(x,0) = \phi(x)$ for $x \in \Omega$, and boundary condition $u(x,t) = 0$ for $x \in \partial\Omega, t \in (0,T)$. In this IBVP, the Caputo fractional derivative D_t^α is defined by $D_t^\alpha g(x,t) := \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t} (t-s)^{-\alpha} \frac{\partial g(x,s)}{\partial s} ds$ for $(x,t) \in Q$.

The use of fractional derivatives in the modelling of various physical processes has grown spectacularly in the last 10 years, and the above IBVP has been considered in many recent numerical analysis papers. A fundamental attribute of the problem is that, even when the data of the problem are smooth and compatible, typical solutions exhibit a weak singularity at the initial time $t = 0$: for each fixed x and $\ell = 1,2,\ldots$, the partial derivatives $\partial^\ell u(x,t)/\partial t^\ell$ blow up as $t \to 0^+$, which complicates significantly the construction and analysis of numerical methods for solving IBVP.

We consider what happens to the IBVP if one (formally) takes the limit $\alpha \to 1^-$; this limit is of great interest since fractional-derivative models are generally perturbations of classical models where $\alpha = 1$. Thus, define the parabolic IBVP $\frac{\partial v}{\partial t} - p\Delta u + c(x)v = f(x,t)$ for $(x,t) \in Q$, with initial condition $v(x,0) = \phi(x)$ for $x \in \Omega$, and boundary condition $v(x,t) = 0$ for $x \in \partial\Omega, t \in (0,T)$. Unlike the solution u of the original IBVP, the solution v of the parabolic IBVP has no singularity at $t = 0$, given sufficient smoothness and compatibility of the data. Furthermore, one can show [1, Theorem 2.5] that $\lim_{\alpha \to 1^-} \max_{(x,t) \in Q} |u(x,t) - v(x,t)| = 0$. That is, as $\alpha \to 1^-$, the solution of the original IBVP approaches the solution of the parabolic IBVP at all points in the space-time domain.

But when we examine the theoretical convergence results in those numerical analysis papers that consider our IBVP, we find — surprisingly — that in most papers, the error bounds obtained blow up as $\alpha \to 1^-$, even though there is no "blow-up" behaviour in the IBVP as $\alpha \to 1^-$. This happens for a variety of numerical methods and a variety of norms.

Note however that our experiments with several numerical methods show that the computed solutions of the original IBVP converge to the computed solutions of the parabolic IBVP as $\alpha \to 1^-$. Thus this blow-up phenomenon is a weakness of the error analyses, not a weakness of the numerical methods.

Our paper [1] exhibits theoretical error bounds from several papers where this unnatural blow-up phenomenon appears, and in some cases is able to offer improved error analyses that derive error bounds that do not blow up in this way. The paper has drawn the attention of several researchers to this anomaly in the research literature, and has stimulated research into improving current error analyses. Google Scholar indicates that the paper [1], which appeared only recently, already has 15 citations.

时间分数阶初边值问题爆破的误差估计

(陈虎，**Martin Stynes***)

对固定的 $\alpha \in (0,1)$，我们考虑时间分数阶初边值问题（IBVP）$D_t^\alpha u - p\Delta u + c(x)u = f(x,t)$，$(x,t) \in Q := \Omega \times (0,T)$，其中 Ω 表示在 $\mathbb{R}^d$ 上的边界区域且 $d \in \{1,2,3\}$，并满足初值条件 $u(x,0) = \phi(x),\ x \in \Omega$，和边值条件 $u(x,t) = 0,\ x \in \partial\Omega, t \in (0,T)$。在 IBVP中，Caputo分数阶导数 D_t^α 定义式为

$$D_t^\alpha g(x,t) := \frac{1}{\Gamma(1-\alpha)} \int_{s=0}^{t} (t-s)^{-\alpha} \frac{\partial g(x,s)}{\partial s} ds$$

在过去的10年里，分数阶导数在各种物理过程建模中的应用有了惊人的增长。上述IBVP在最近的许多数值分析论文中都得到了考虑，该问题的一个基本属性是：即使问题的数据是光滑的和兼容的， 问题的解在初始时刻 $t = 0$: 处具有弱奇异性，也就是说对于固定的 x 和 $\ell = 1,2,\ldots$，$\partial^\ell u(x,t)/\partial t^\ell$ 会随着 $t \to 0^+$ 而爆破，这大大增加了IBVP数值方法构造和分析的复杂性。

我们考虑如果（形式上）取极限 $\alpha \to 1^-$，IBVP会发生什么？由于分数导数模型通常是 $\alpha = 1$ 的经典模型的扰动，所以这个极限是非常有趣的。因此，我们定义抛物型IBVP $\frac{\partial v}{\partial t} - p\Delta u + c(x)v = f(x,t)$，$(x,t) \in Q$, 满足初值条件 $v(x,0) = \phi(x),\ x \in \Omega$，和边值条件 $v(x,t) = 0,\ x \in \partial\Omega, t \in (0,T)$。与原始IBVP的解 u 不同，抛物型IBVP的解 v 在数据给定的足够的光滑性和兼容性的情况下，在初始时刻 $t = 0$ 处没有弱奇异性。 此外，通过 [1, Theorem 2.5] 可知 $\lim_{\alpha \to 1^-} \max_{(x,t)\in\bar{Q}} |u(x,t) - v(x,t)| = 0$。 也就是说，当 $\alpha \to 1^-$ 时，原始IBVP的解在时空区域中的所有点上都趋于抛物型IBVP的解。

但是，当我们检查那些考虑我们的IBVP的数值分析论文中的理论收敛结果时，我们惊奇地发现，在大多数论文中得到的误差边界在 $\alpha \to 1^-$ 时会爆破，即使IBVP在 $\alpha \to 1^-$ 时没有“爆破”行为，这发生在各种数值方法和各种范数中。

值得注意的是，我们用几种数值方法进行的实验表明，原始IBVP的数值解在 $\alpha \to 1^-$ 时收敛于抛物型IBVP的数值解。因此，这种爆破现象是误差分析的弱点，而不是数值方法的弱点。

我们的论文[1]展示了出现这种非自然爆破现象的几篇论文中的理论误差界限，并且在某些情况下能够提供改进的误差分析，可得出不以这种方式爆破的误差界限。本文的研究引起了一些研究人员对这一异常现象的注意，并促进了改进当前误差分析的研究。谷歌Scholar指出，我们最近才发表的论文[1]已经被引用了15次。

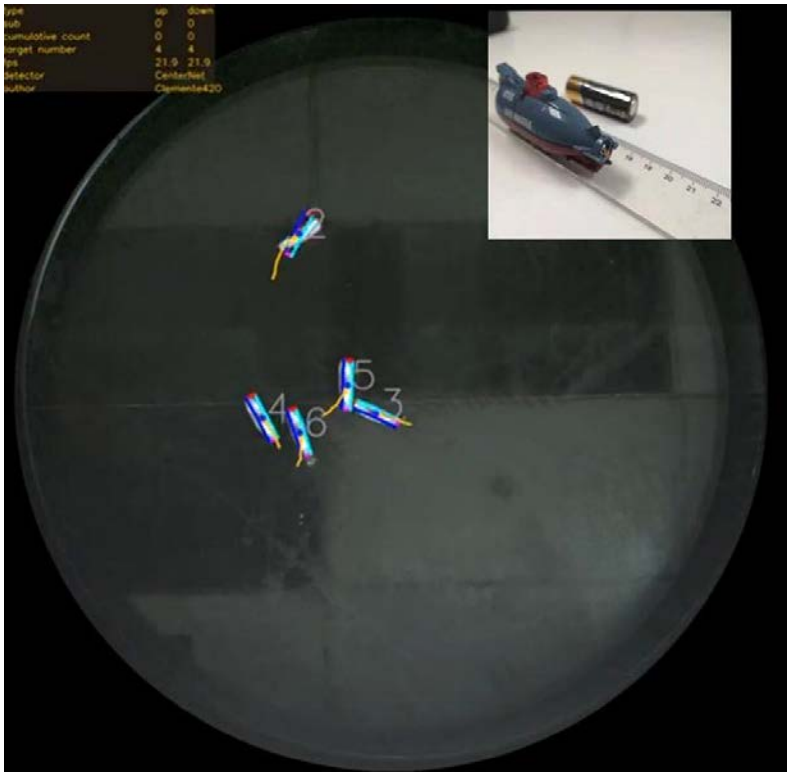
References:

[1] Hu Chen & Martin Stynes, Blow-up of error estimates in time-fractional initial-boundary value problems, IMA J. Numer. Anal. 41 (2021), 974–997. DOI: 10.1093/imanum/draa015

A ROBOTIC PLATFORM FOR STUDYING COLLECTIVE MOTION IN WATER

(By **Rong Fu**, **Yang Ding**, **Xinliang Xu**)

With limited ability at individual level, some organisms at large number have complex behavior and intelligence that seems to be far beyond any individual. For example, some fish species swim together to avoid prey and dolphins sometime collaborate to prey fish. How such phenomena emerge and the underlying mechanisms have been one of the central topics of complexity studies. With the rapid development of robotic technology, researchers have been trying to make robots collaborate and accomplish complex and difficult tasks. Previous studies have shown that complex schooling behaviors can be produced by simple control strategies by each individual and hydrodynamical interactions [1]. However, the hydrodynamic interactions in previous studies are captured by simple and idealized models because accurate simulation of hydrodynamic interactions between many swimmers is computationally infeasible. On the other hand, experimental study of large number of current underwater autonomous vehicles (UAVs) requires huge resources.



A team led by Yang Ding from CSRC developed a table-top experimental platform for studying the underwater collective behavior. They chose toy submarines as the robotic swimmers, since those toy submarines are cheap, small (7.5cm long), and reliable. They modified the control system such that each toy submarine can be controlled individually and quickly. The time to give each submarine a command for 100 submarines is within a second. They put the toy submarines into a round pool with 1.2m diameter and monitored by a camera on top. They developed a tracking software based on open-source object detection packages and pattern matching packages. With the tracking hardware and software, they are able to obtain the positions, orientations and velocities of the toy submarines. With such a system, they began to test simple strategies with hydrodynamic interactions. As shown in the figure, four swimmers are following a leading swimmer. In future, they plan to test previously proposed models and mechanisms for collective behaviors exhibited by animals as well as strategies for swarm robots.

水下集群运动的机器人研究平台

（付蓉，丁阳，徐辛亮）

由个体的能力有限的个体组成的集群生物具有复杂的行为和智力，通常远远超出任何个体。比如，为了躲避天敌，许多鱼类会成群结队的一起游动，海豚还会通过合作捕食猎物。这些现象是如何出现以及其潜在的机制一直是复杂性研究的核心主题之一。随着机器人技术的发展，研究人员开展了大量的研究工作，以使机器人通过相互合作来完成复杂且困难的任务。以往的研究表明，复杂的群体行为可以通过个体的简单控制策略和流体动力相互作用产生[1]。然而，由于精确地模拟多游泳者之间的水动力相互作用在计算上不可行的，因此以往的研究中地水动力相互作用都是通过简单的理想化模型以模拟。另一方面，大量的水下自组织机器人的实验研究需要许多资源支持。

由北京计算科学研究中心的丁阳领导的团队开发了研究水流环境中集体行为的桌面实验平台。他们选择玩具潜艇作为机器人游泳者，因为这些玩具潜艇便宜、小(7.5厘米长)且可靠。改进了玩具潜艇的控制系统，使每艘玩具潜艇都能被单独快速地控制，可以在一秒钟之内给100艘潜艇的每艘潜艇下达相应指令。他们将多个玩具潜艇放入直径1.2米的圆形水池中，用顶部的摄像机监控，并且开发了一个基于开源目标检测包和模式匹配的跟踪软件包。通过硬件和软件进行跟踪，能够获得玩具潜艇的位置、方向和速度。通过这个系统，他们开始用简单的策略来测试流体相互作用。如图所示，四个机器人游泳者跟随一个领导的游泳者运动。未来，他们计划测试之前提出的动物集体行为模型和机制，以及群体机器人的策略。

References:

[1] Filella, Audrey, François Nadal, Clément Sire, Eva Kanso, and Christophe Eloy. "Model of collective fish behavior with hydrodynamic interactions." Physical review letters 120, no. 19 (2018): 198101.

A DIFFUSE DOMAIN METHOD FOR TWO-PHASE FLOWS WITH LARGE DENSITY RATIO IN COMPLEX GEOMETRIES

(By **Zhenlin Guo**, Fei Yu, Ping Lin, Steven Wise and John Lowengrub)

Zhenlin Guo et al. present a quasi-incompressible Navier–Stokes–Cahn–Hilliard (q-NSCH) diffuse interface model for two-phase fluid flows with variable physical properties that maintains thermodynamic consistency. Then, they couple the diffuse domain method with this two-phase fluid model – yielding a new q-NSCH-DD model – to simulate the two-phase flows with moving contact lines in complex geometries. The original complex domain is extended to a larger regular domain, usually a cuboid, and the complex domain boundary is replaced by an interfacial region with finite thickness. A phase-field function is introduced to approximate the characteristic function of the original domain of interest. The original fluid model, q-NSCH, is reformulated on the larger domain with additional source terms that approximate the boundary conditions on the solid surface. They show that the q-NSCH-DD system converges to the q-NSCH system asymptotically as the thickness of the diffuse domain interface introduced by the phase-field function shrinks to zero with first order. Our analytic results are confirmed numerically by measuring the errors in both L_2 and L_inf norms. In addition, we show that the q-NSCH-DD system not only allows the contact line to move on curved boundaries, but also makes the fluid–fluid interface intersect the solid object at an angle that is consistent with the prescribed contact angle.

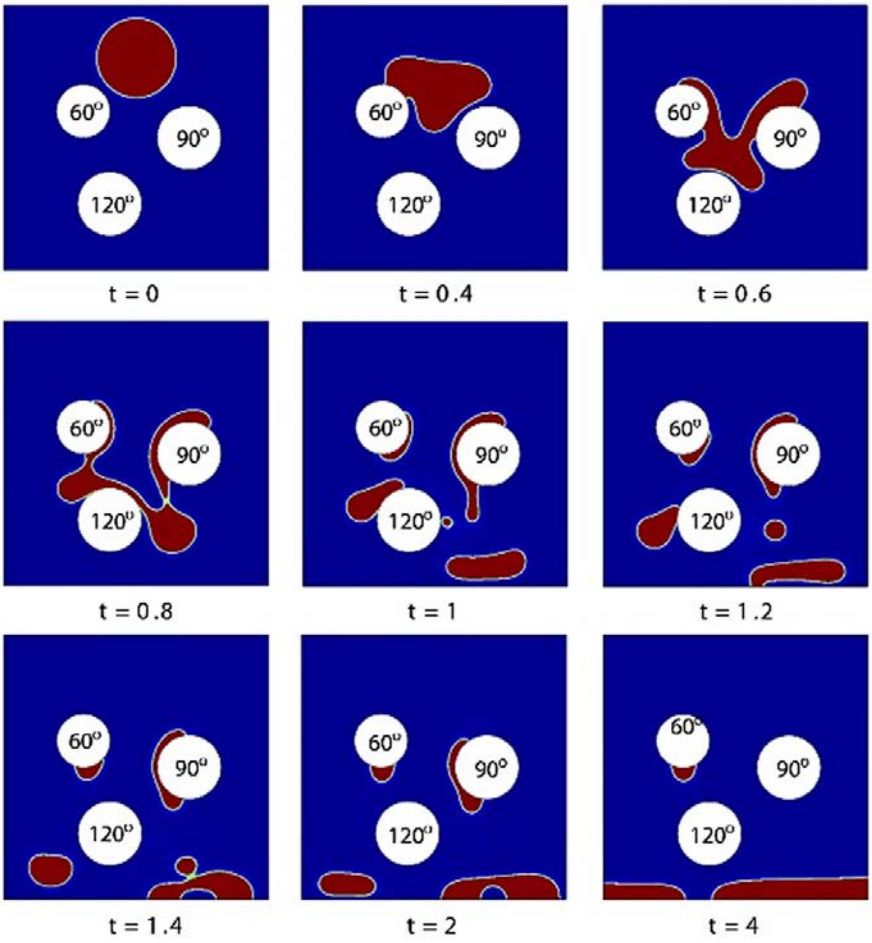


Fig. 1. Snapshots of the penetration of liquid droplet into porous media with different static contact angle, where the angles are indicated inside the white cylinders.

扩散区域法：一类用来求解复杂区域偏微分方程的数值算法

（郭震林，Fei Yu，Ping Lin, Steven Wise and John Lowengrub）

在这篇文章中，郭震林及合作者一同发展了一个用来在复杂区域内求解偏微分方程的数值算法：扩散区域法。这个方法是基于相场模型，通过引入一个相场变量Phi，将原来的复杂区域扩充到一个更大的规则区域内，之后使用相场变量，标记原复杂区域。即：这个相场变量Phi，在原区域内取值1，在扩充的额外区域部分取0，在复杂边界上，相场变量连续且快速的从0过渡1，并引入一个小参数epsilon控制过渡区域的厚度。原偏微分方程，就通过扩散区域法的格式与相场变量Phi进行耦合，被扩充到了更大的规则区域内，原来在复杂区域上满足的边界条件也被改写为源项，放在新的方程右端。求救新的方程，只需在规则区域内进行求解，这样就避免了对于复杂区域边界的处理。郭震林及合作者一起，应用扩散区域法，数值模拟了多相流在复杂区域内流动的问题。并通过渐进分析，证明了算法精度，并进行了数值验证。

◀ 图 1　空气中的水滴穿过多空介质的过程。每个圆柱设定了不同的静态接触角。

References:

[1] Zhenlin Guo et al., A diffuse domain method for two-phase flows with large density ratio in complex geometries, J. Fluid. Mech., 2021.

HERMITE SPECTRAL METHOD FOR FOKKER-PLANCK-LANDAU EQUATION MODELING COLLISIONAL PLASMA

(By Ruo Li , Yinuo Ren, **Yanli Wang***)

The Fokker-Planck-Landau (FPL) equation is used to describe the evolution of collisional plasma systems at the kinetic level. It is a six-dimensional integro-differential equation, which models binary collisions between charged particles with long-range Coulomb interactions. The FPL equation is the limit of the Boltzmann equation when all binary collisions are grazing. It was originally derived by Landau and was later derived independently in the Fokker-Planck form. The high-dimensionality of the FPL equation is a bottleneck for its numerical simulations. Although several simplified models of the original FPL equation has been developed, it is still a challenge to solve it both fast and accurately.

One of the major difficulties in solving FPL equation numerically is the complexity of the Fokker-Planck collision operator, which is an integro-differential nonlinear operator in the microscopic velocity space. Most of the statistical methods, such as the DSMC method, are limited for the FPL equation since the FPL collision operator models the infinite-range potential interactions within the plasma. Several deterministic methods are used to solve the FPL equation or its simplifications. The entropic scheme, which guarantees a nondecreasing entropy, is well studied. To handle the stiffness of the collision operator, an asymptotic-preserving (AP) strategy is studied, while a conservative spectral method is also adopted. A positivity-preserving scheme for the linearized FPL equation is proposed, after which it was modified to preserve energy and then extended to the two-dimensional FPL equation with cylindrical geometry. Several other numerical methods, such as the multipole expansions and multigrid techniques have also been proposed. The finite element methods and the semi-Lagrangian schemes are also used to solve the Vlasov equations.

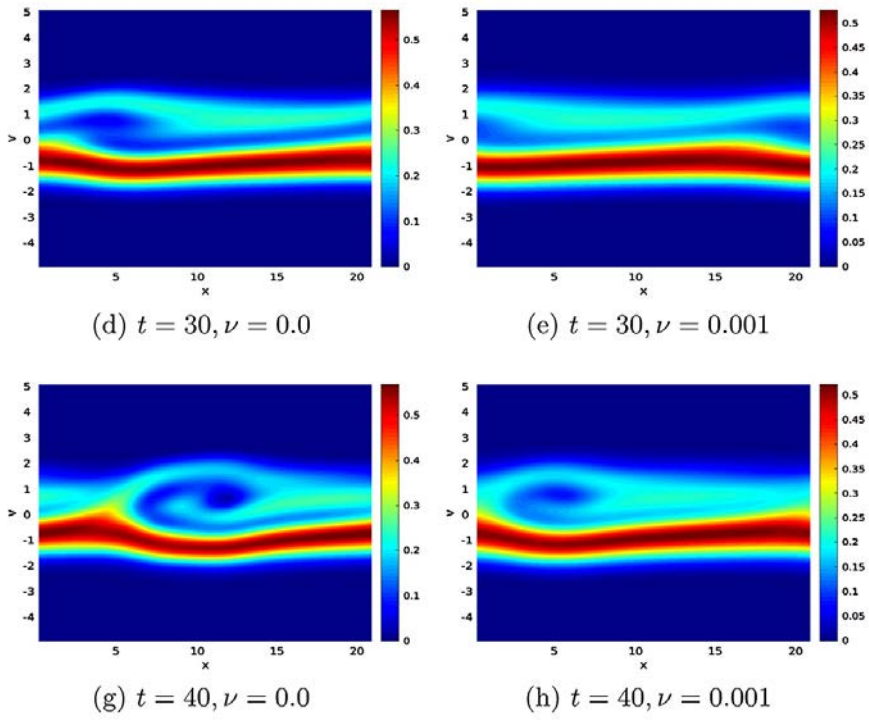


Fig. 1. Bump on tail problem.

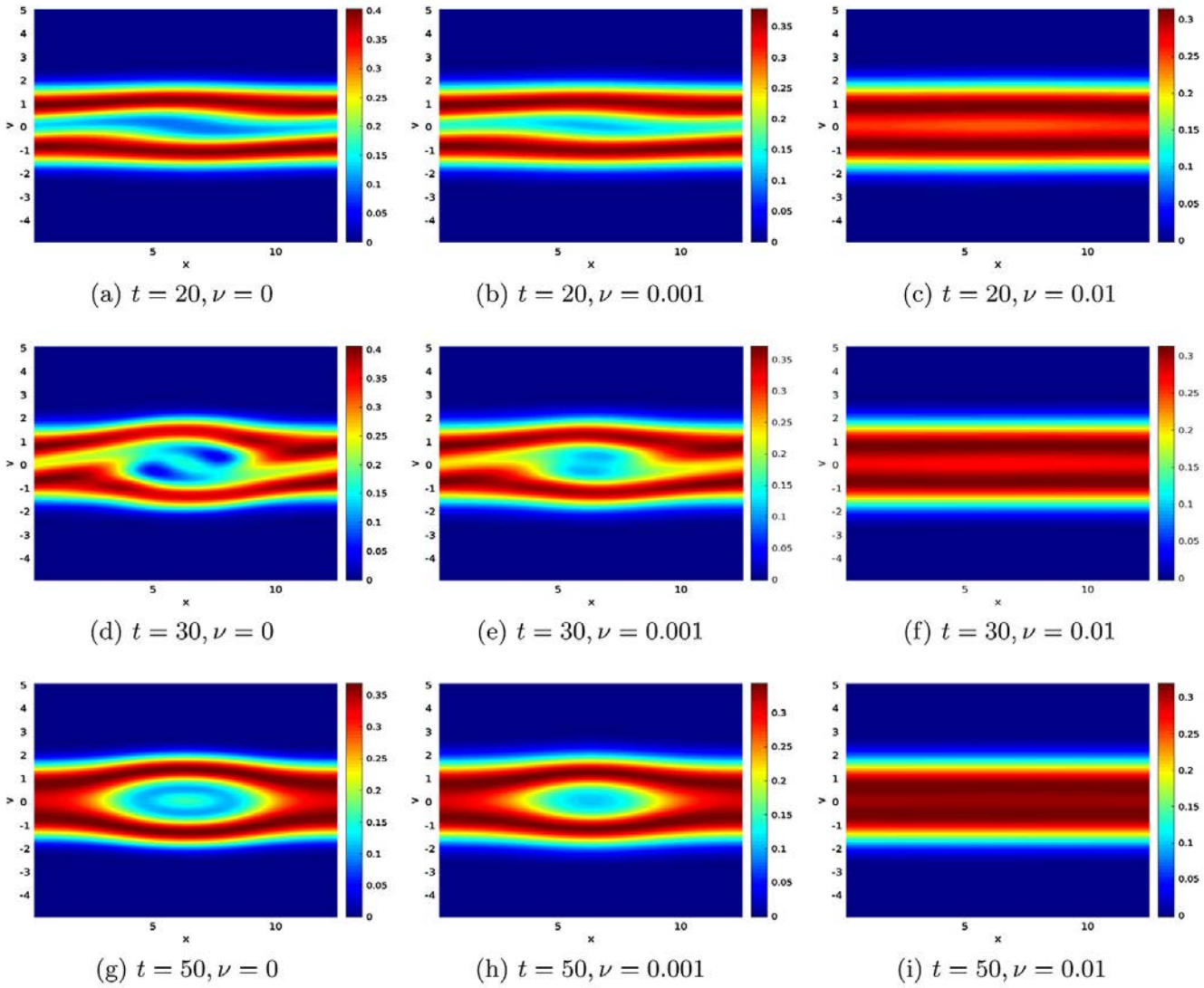


Fig. 2. Two stream flow.

In this work, we propose an Hermite spectral method for the Fokker-Planck-Landau (FPL) equation. Both the distribution functions and the collision terms are approximated by series expansions of the Hermite functions. To handle the complexity of the quadratic FPL collision operator, a reduced collision model is built by adopting the quadratic collision operator for the lower-order terms and the diffusive Fokker-Planck operator for the higher-order terms in the Hermite expansion of the reduced collision operator. The numerical scheme is split into three steps according to the Strang splitting, where different expansion centers are employed for different numerical steps to take advantage of the Hermite functions. The standard normalized Hermite basis is adopted during the convection and collision steps to utilize the precalculated coefficients of the quadratic collision terms, while the one constituted by the local macroscopic velocity and temperature is utilized for the acceleration step, by which the effect of the external force can be simplified to an ODE. Several numerical examples such as the bump on tail problem and the two stream flow are studied to test and validate our new method.

Fokker-Planck-Landau方程模型下碰撞等离子体的Hermite谱方法

（李若，任一诺，**王艳莉***）

Fokker-Planck-Landau方程是一个被广泛用来在动理学层面描述碰撞等离子体系统演化的方程，其形式为七维积分-微分方程。Fokker-Planck-Landau方程描述了长距离Coulomb力作用下带电粒子的二元碰撞，是Boltzmann方程在所有二元碰撞趋近于掠射时的极限。Fokker-Planck-Landau方程首先被Landau提出，其 Fokker Planck形式在之后又被独立提出。Fokker-Planck-Landau方程的高维性是其数值模拟的主要瓶颈，因此尽管已经有很多对于原始的Fokker-Planck-Landau 方程的简化模型提出，对Fokker-Planck-Landau方程进行既快速又准确的数值求解依然是一件非常困难的工作。

Fokker-Planck-Landau碰撞算子是一个微观速度空间中的非线性积分-微分算子，其复杂性是数值求解Fokker-Planck-Landau方程中最重要的难点之一。因为 Fokker-Planck碰撞算子描述的是等离子体中无穷距离的势能作用，所以大部分的统计方法, 诸如DSMC方法，在数值求解Fokker-Planck-Landau方程上都遇到了困难。很多确定性方法被用来数值求解Fokker-Planck-Landau方程或其简化形式，保证熵不减的熵格式（entropy scheme）也在此类问题上被广泛研究。为了处理Fokker-Planck碰撞算子的刚性，人们提出了一种渐近保持（asymptotic-preserving）的策略来处理本问题。保正（positivity-preserving）格式被用来数值求解线性化的Fokker-Planck-Landau方程，该格式后来被改良以保证能量守恒，并在之后被进一步发展用来数值求解二维圆柱几何（cylindrical geometry）的Fokker-Planck-Landau方程。一些其他的数值算法，比如多极（multipole）展开与多重网格 （multigrid）技巧，也被广泛应用于此类问题。一种完全隐式的格式算法被用来数值求解多维的Rosenbluth-Fokker-Planck方程。有限元方法与Semi-Lagrangian方法也被用来数值求解Vlasov方程。此

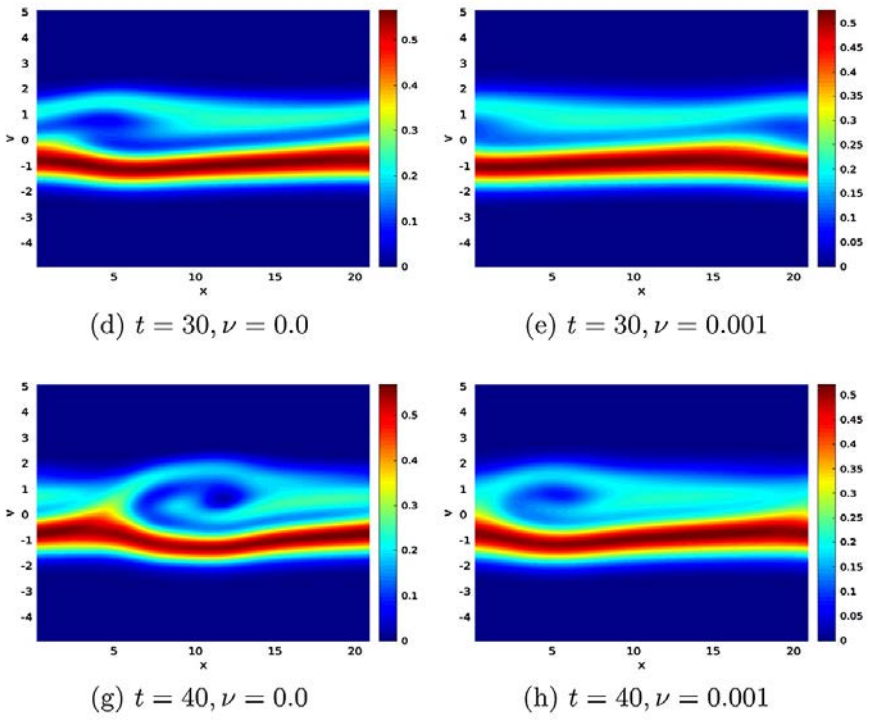


Fig. 1. Bump on tail problem.

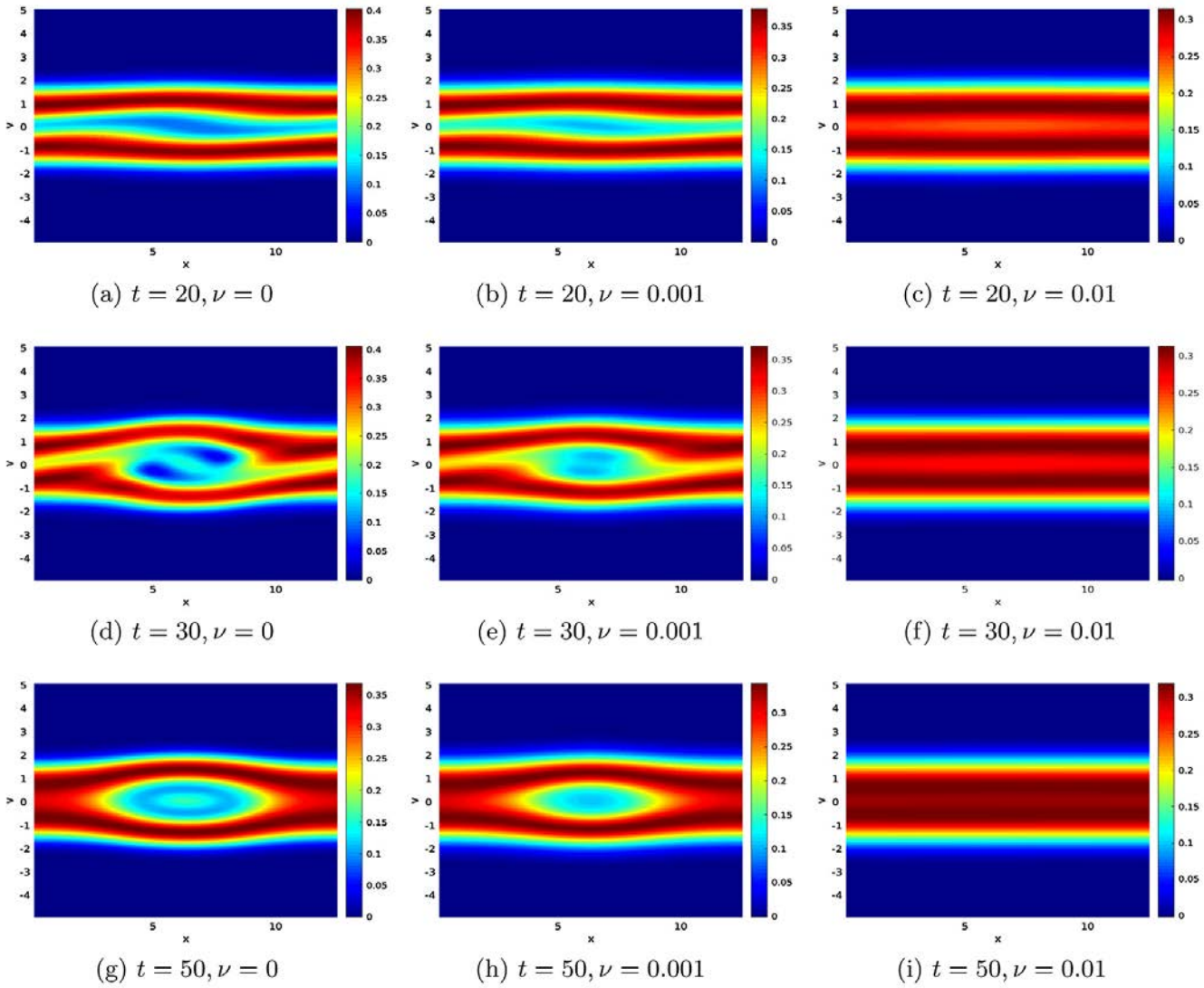


Fig. 2. Two stream flow.

外，带有随机性的 Fokker-Planck-Landau 方程也已经被探讨。

在本论文中，我们为空间非均匀的Fokker-Planck-Landau方程提出了一种Hermite 谱方法。在本谱方法中，分布函数与碰撞项均以Hermite函数为基进行级数展开，并以该级数展开作为其近似。为了处理二次Fokker-Planck-Landau算子的计算复杂性，我们构建了一种简化碰撞模型。在该模型的低阶项中采用二次碰撞算子、高阶项中采用扩散Fokker-Planck算子。根据Strang分裂法，数值格式分为对流、加速与碰撞三个相继的数值步。在对流与碰撞步中，我们采取标准Hermite展开，从而充分应用我们在过去工作中得到的二次碰撞项系数；在加速步中，展开中心被选取为局部宏观速度与温度，从而外力的作用被简化为一个易于计算的常微分方程。我们测试了线性Landau阻尼的算例，并研究了其中静电能的衰减速率与碰撞速率的关系。此外，双流不稳定性与Bump-on-tail不稳定性的模拟也进一步证实我们提出的数值算法的有效性。

ATOMISTIC DESIGN OF LOW THERMAL CONDUCTIVITY IN 2D MATERIALS

(By **Zhen Tong**, Alessandro Pecchia, **ChiYung Yam**, Traian Dumitrică,* and **Thomas Frauenheim***)

Materials with ultrahigh or low thermal conductivity are desirable for many technological applications, such as thermal management of electronic and photonic devices, heat exchangers, energy converters and thermal insulation. Recent advances in simulation tools (first principles, the atomistic Green's function and molecular dynamics) and experimental techniques (pump–probe techniques and microfabricated platforms) have led to new insights on phonon transport and scattering in materials and the discovery of new thermal materials, and are enabling the engineering of phonons towards desired thermal properties. Particularly, Frauenheim group here focus on the strategies for designing and screening low thermal conductivity in two-dimensional (2D) materials including: 1) ultralow thermal conductivity in two-dimensional molybdenum trioxide (MoO_3) with intrinsic strong anharmonicity through mechanisms like soft out-of-plane phonon modes [1], and 2) significant suppression of phononic thermal transport along Graphene grain boundaries (GBs)

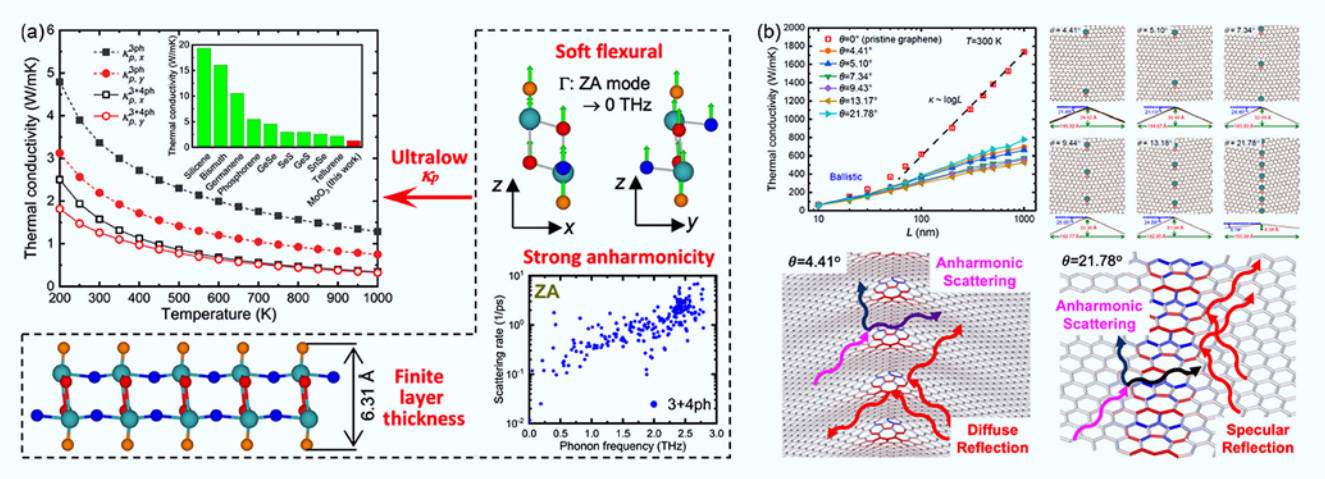


Fig. 1. (a) Temperature-dependent thermal conductivity of two-dimensional MoO3. The structure of finite layer thickness of 2D MoO_3 with its lattice vibrational pattern and the three- and four-phonon scattering rates of the out-of-plane acoustic phonon modes (ZA). (b) Length-dependent thermal conductivity along Graphene GBs. The structure of different GBs with the periodic GB strain field, which behaves as a reflective diffraction grating with either diffuse or specular phonon reflections.

with extrinsic enhanced phonon scattering through spectral phonon engineering [2]. First, monolayer MoO_3 is an emerging 2D material with high electrical conductivity but unexplored thermal conductivity. Using first-principles calculations and a Boltzmann transport theoretical framework, they predict a record low room-temperature phonon thermal conductivity of 1.57 and 1.26 W/mK along the principal in-plane directions of the MoO_3 monolayer. The behavior is attributed to the combination of soft flexural and in-plane acoustic modes, which are coupled through the finite layer thickness, and to the strong bonding anharmonicity, which gives rise to significant 3- and 4-phonon scattering, as shown in Fig. 1(a). These insights suggest new indicators for guiding the search of 2D materials with low thermal conductivity

图 1　(a) 二维MoO3随温度变化的热导率，以及有限层厚度原子结构及其面外声子(ZA)晶格振动模式和三声子、四声子散射率。(b)沿石墨烯晶界的长度依赖性热导率关系，以及不同的石墨烯晶界结构和其周期性晶界应变场中的漫反射或镜面声子反射及非简谐声子散射的反射衍射光栅示意图。

低热导率二维材料的原子尺度模拟设计

（童贞，Alessandro Pecchia，任志勇，Traian Dumitric ă *，**Thomas Frauenheim***）

许多技术应用都需要具有超高或低热导率的材料，例如电子和光子设备的热管理、热交换器、能量转换器和隔热。数值模拟计算工具(例如第一原理、原子格林函数和分子动力学等)和实验技术(泵-探针技术和微制造平台等)的最新进展促进了对材料中声子传输和散射的新见解以及新热材料的发现，以及正在使声子工程来调控达到所需的热特性。Frauenheim研究组在这里重点关注设计和筛选二维材料中的低热导率的策略，包括：1)二维三氧化钼(MoO_3)中的超低热导率主要源于其内在的强非谐性平面声子模式[1]；2) 沿石墨烯晶界方向的声子热导率的显着降低主要是由于位错缺陷导致的局部声子散射[2]。首先，单层MoO_3是一种新兴的二维材料，具有高电导率但尚未研究其热导率。在这里通过第一性原理计算并结合玻尔兹曼输运理论框架，他们发现单层MoO3在面内具有超低的声子热导率，室温下分别为1.57和1.26 W/mK。这主要归因于软化的面外声学声子模和平面内声学模式的强耦合散射，它们通过有限的层厚度耦合，以及强键非简谐性，导致了很强的的三声子和四声子散射，如图1(a)所示。这些见解为指导寻找低导热率的二维材料提供了新的指标，并推动了对二维MoO_3热物性的实验测量以及将其作为热电和热保护材料的应用。另外，尽管石墨烯晶界在实验上得到了很好的表征，但它们对其热传输特性的影响却鲜为人知。正如这里所揭示的，即使晶界在超窄石墨烯纳米带种并沿着温度梯度方向排列，其热传输也很容易受到晶界的影响。他们利用非平衡分子动力学模拟揭示了石墨烯中沿着线性变化的晶界(周期性重复的五边形-七边形位错)的声子热导率大幅降低。同时，格林函数计算和光谱能量密度分析表明，热导率降低的起源隐藏在周期性晶界应变场中，它表现为具有漫反射或镜面声子反射的反射衍射光栅，也是非简谐声子-声子散射的局域化散射源，如图1(b)所示。然而经典的Klemens理论无法解释此处揭示的热导率与位错密度的非单调相关性，他们的工作可以帮助理论指导设计出能够最好地保持声子传输完整性的晶界结构。

References:

[1] Zhen Tong, Traian Dumitrică*, and Thomas Frauenheim*, Ultralow thermal conductivity of two-dimensional MoO_3, Nano Letters, 21, 4351–4356, 2021.

[2] Zhen Tong, Alessandro Pecchia, ChiYung Yam, Traian Dumitrică*, and Thomas Frauenheim*, Phononic thermal transport along graphene grain boundaries: A Hidden Vulnerability, Advanced Science, 2101624, 2021.

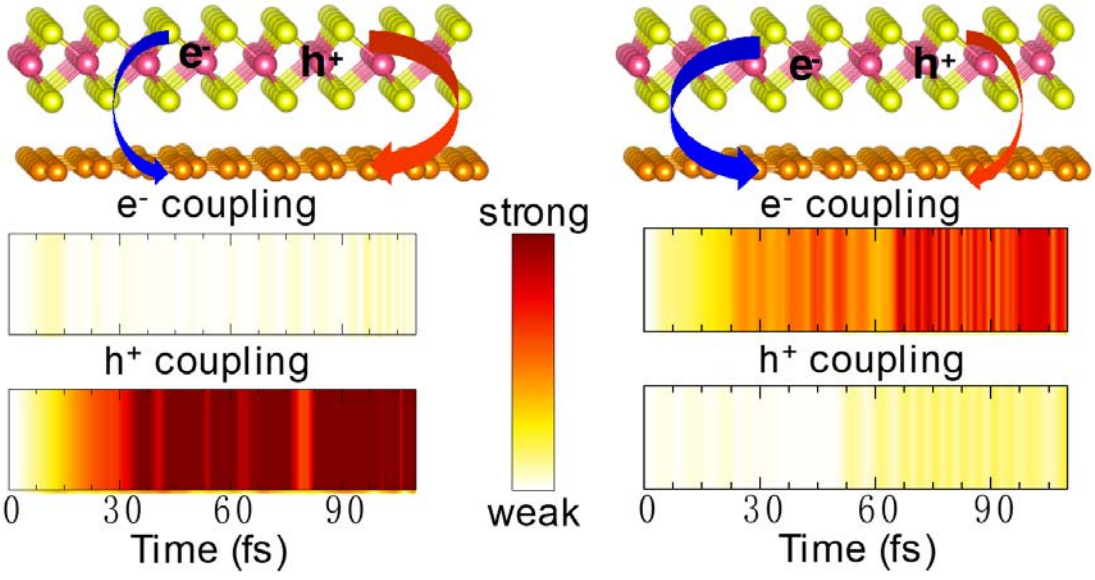
and motivates the measurements in MoO_3 and its applications as a thermoelectric and thermally protective material. Second, while graphene GBs are well characterized experimentally, their influence on transport properties is less understood. As revealed here, phononic thermal transport is vulnerable to GBs even when they are ultra-narrow and aligned along the temperature gradient direction. Non-equilibrium molecular dynamics simulations uncover large reductions in the phononic thermal conductivity along linear GBs comprising periodically repeating pentagon-heptagon dislocations. Green's function calculations and spectral energy density analysis indicate that the origin of the thermal conductivity reduction is hidden in the periodic GB strain field, which behaves as a reflective diffraction grating with either diffuse or specular phonon reflections, and represents a source of anharmonic phonon–phonon scattering, as shown in Fig. 1(b). The non-monotonic dependence with dislocation density of thermal conductivity uncovered here is unaccounted for by the classical Klemens theory. It can help identify GB structures that can best preserve the integrity of the phononic transport.

ELECTRIC FIELD TUNABLE ULTRAFAST INTERLAYER CHARGE TRANSFER IN GRAPHENE/WS2 HETERSTRUCTURE

(By Yuxiang Liu and **ChiYung Yam**)

In the past few years, vertical van der Waals heterostructures composed of two-dimensional (2D) materials have attracted tremendous attentions[1]. Graphene/TMDCs heterostructure has been taken as promising materials for optoelectronics due to its high electrical conductivity and superior light-absorption property. Many experimental and theoretical efforts have been made to ultrafast charge transfer process at heterointerfaces[2, 3].

ChiYung Yam *et al*. at Beijing Computational Science Research Center take advantage of external electric field to tune charge transfer and investigate the mechanism and modulation of charge dynamics. They employed real-time time-dependent density functional theory combined with non-adiabatic molecular dynamics to investigate charge transfer in graphene/WS2 heterostructure. The results demonstrate that photoexcited hole transfer from WS2 to graphene more efficiently than electrons. The ultrafast charge transfer arises from the coupling to the nuclear vibration of graphene and WS_2 and its amplitude and polarity show a strong dependence on the external electric fields. Further analysis reveals that the interlayer charge transfer process in graphene/WS_2 is governed by the coupling between carriers and the final states, in other words, it is the result of the competition between carrier interlayer and intralayer relaxation process. This work is published in *Nano Lett*. 21, 4403-4409 (2021).



通过外加电场实现的石墨烯/二硫化钨异质结的可调电荷转移

（刘宇翔，任志勇）

近年来，由二维材料组成的范德华异质结因其独特的电学和光学性质引起了广泛关注。具有高电导率和高光吸收的等特点石墨烯/过渡金属二硫化物异质被视为应用前景广泛的光电器件材料[1]。超快电荷转移过程作为异质结实际应用的关键吸引了大量的实验和理论研究。最近，实验中发现光激发的空穴和电子可以快速从二硫化钨转移到石墨烯中，并且空穴转移的速度远超电子转移的速度。因此，对于电荷转移的机理的理论研究以及进一步调控电荷转移过程，对异质结材料在光电器件方面的应用具有重要作用[2,3]。

来自北京计算科学研究中心的任志勇等研究人员利用外加电场调控石墨烯/二硫化钨异质结界面的电荷转移过程，研究了异质结中电荷转移的机理以及器件中电荷转移的可控性。他们利用含时密度泛函理论结合非绝热分子动力学的方法，对电荷转移过程进行模拟。结果表明，石墨烯/二硫化钨异质结中光激发的空穴转移快于电子转移。而超快电荷转移的过程与石墨烯和二硫化钨的原子振动模有关，并且可以通过外加电场调控电荷转移的速度以及方向。进一步的分析表明，异质结中的层间电荷转移过程是层间电荷转移与层内电荷转移的竞争结果，而这个过程是由电荷与接收态之间的耦合强度决定的。因此，可以通过调节外加电场来调节电荷与接收态之间的耦合强度，实现对电荷转移过程的控制。这些发现为异质结材料在光电器件方面的实际应用提供了参考。该工作发表在*Nano Lett*. 21, 4403-4409 (2021).

References:

[1] Choi, W., Mater. Today 20.3 (2017): 116-130.
[2] Li, Y., Adv. Funct. Mater. 26.24 (2016): 4319-4328.
[3] Aeschlimann, S., Sci. Adv. 6.20, eaay0761(2020).

2020-2021学术年期间，中心承担中央组织部、科学技术部、国家基金委、博士后科学基金，以及中物院等在研项目共123项，其中年内结题44项。另外，2021年8月后中心将新启动项目12项。

During the 2020-2021 academic year, CSRC is undertakeing 123 projects from the Ministry of Science and Technology of China, National Natural Science Foundation of China, China Academy of Engineering Physics, China Postdoctoral Science Foundation and so on. 44 projects were concluded during the academic year. In addition, 12 new projects will be started after August 2020.

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
1	林海青	科学技术部	国家重点研发计划	低维固态极性结构中量子态调控及其原型器件研究	2017.07 - 2022.06
2	游建强	科学技术部	国家重点研发计划	高品质腔与固体量子态的耦合及其量子调控	2016.07 - 2021.06
3	黄　兵	军委科技委	基础加强计划重点基础研究项目	非平衡态下半导体材料缺陷的基础科学问题研究	2018.01 - 2021.12
4	管鹏飞	国防科技工业局	国防基础科研核科学挑战专题	辐照条件多尺度计算与模拟研究	2018.01 - 2021.12
5	魏苏淮	北京市科学技术委员会	—	铜铟镓硒电池的碱金属后处理及相关技术研究	2018.06 - 2021.05
6	胡淑贤	中国工程物理研究院	院长基金	锕系化合物的多组态量子化学研究	2018.01 - 2020.12
7	林海青	国家自然科学基金委员会	联合基金项目	科学计算与物理系统模拟研究	2020.01 - 2022.12
8	赵　楠	国家自然科学基金委员会	联合基金项目重点项目	基于原子自旋的惯性传感物理基础与小型化系统综合优化研究	2021.01 - 2024.12
9	魏苏淮	国家自然科学基金委员会	重大项目	微纳器件中非平衡物理过程研究	2020.01 - 2024.12
10	孙昌璞	国家自然科学基金委员会	重点项目	有限开放系统的量子相干效应及其应用	2016.01 - 2020.12
11	魏苏淮	国家自然科学基金委员会	重点项目	透明导电体的物理机理研究与新材料设计	2017.01 - 2021.12

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
12	汤雷翰	国家自然科学基金委员会	重点项目	活性系统的热耗散及长时动力学	2017.01 - 2021.12
13	林海青	国家自然科学基金委员会	重点项目	海森堡模型和Kitaev模型的元激发、激发谱和量子相变	2018.01 - 2022.12
14	高世武	国家自然科学基金委员会	重点项目	表面激发态和非绝热动力学方法及应用	2020.01 - 2024.12
15	张智民	国家自然科学基金委员会	重点项目	偏微分方程特征值问题的特征适应型算法与理论	2022.01 - 2026.12
16	薛　鹏	国家自然科学基金委员会	国家杰出青年科学基金	量子行走的理论与实验研究	2021.01 - 2025.12
17	任志勇	国家自然科学基金委员会	中德合作交流项目	有机-无机混合异质结构中的非绝热光诱导量子动力学	2021.01 - 2023.12
18	Rubem Mondaini	国家自然科学基金委员会	国际(地区)合作与交流项目	平衡及非平衡条件下极化超流体的维度过渡	2021.01 - 2022.12
19	张智民	国家自然科学基金委员会	数学天元基金	麦克斯韦传输特征值问题零散度约束的高效谱方法研究	2020.01 - 2020.12
20	张智民	国家自然科学基金委员会	数学天元基金	Navier-Stokes方程的时空谱元法	2021.01 - 2021.12
21	胡广辉	国家自然科学基金委员会	面上项目	基于固定入射方向的反媒介理论和算法研究	2017.01 - 2020.12
22	丁　阳	国家自然科学基金委员会	面上项目	波状运动中的力矩规律在解释生物驱动控制和设计机器人柔性材料中的应用	2017.01 - 2020.12
23	Rubem Mondaini	国家自然科学基金委员会	面上项目	关联超流体中的赝能隙相变研究	2017.01 - 2020.12
24	张东波	国家自然科学基金委员会	面上项目	低维材料电子性质的应变调控：自洽密度泛函紧束缚广义布洛赫方法	2017.01 - 2020.12
25	任志勇	国家自然科学基金委员会	面上项目	纳米等离子体太阳能电池的光学-电学相结合研究	2017.01 - 2020.12

续表

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
26	魏苏淮	国家自然科学基金委员会	面上项目	复杂半导体清洁能源材料的理论研究	2017.01 - 2020.12
27	张继伟	国家自然科学基金委员会	面上项目	多尺度非局部模型的理论分析和高效数值方法	2018.01 - 2021.12
28	蔡勇勇	国家自然科学基金委员会	面上项目	高振荡色散方程的多尺度计算方法及分析	2018.01 - 2021.12
29	杨　文	国家自然科学基金委员会	面上项目	适用于连续模型的通用格林函数方法及载流子局域输运和干涉现象的理论研究	2018.01 - 2021.12
30	游建强	国家自然科学基金委员会	面上项目	超越玻恩-马科夫近似的固态量子比特系统的量子动力学研究	2018.01 - 2021.12
31	高　翔	国家自然科学基金委员会	面上项目	低能电子-离子散射过程中的Breit效应理论研究	2018.01 - 2021.12
32	李　勇	国家自然科学基金委员会	面上项目	光力系统中光学非互易性传输的理论研究	2018.01 - 2021.12
33	喻　进	国家自然科学基金委员会	面上项目	蛋白因子和分子机器在DNA上的信号探测和信息识别	2018.01 - 2021.12
34	张智民	国家自然科学基金委员会	面上项目	电磁场方程及其特征值问题高效高精度数值方法	2019.01 - 2022.12
35	汪　玲	国家自然科学基金委员会	面上项目	矩阵乘积态的切空间投影法研究强关联系统的自旋动力学结构因子	2019.01 - 2022.12
36	张瑞勤	国家自然科学基金委员会	面上项目	氮化碳表面非金属原子梯度掺杂对光生载流子产生和分离影响的计算研究	2019.01 - 2022.12
37	王　奇	国家自然科学基金委员会	面上项目	热力学一致模型的计算建模保结构算法设计分析与实现	2020.01 - 2023.12
38	徐辛亮	国家自然科学基金委员会	面上项目	活性物质集体运动的涌现及其非平衡态物理特性	2020.01 - 2023.12
39	Rubem Mondaini	国家自然科学基金委员会	面上项目	强关联系统中d波配对的非平衡探索研究	2020.01 - 2023.12

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
40	Stefano Chesi	国家自然科学基金委员会	面上项目	基于半导体量子点的自旋量子比特的长距耦合	2020.01 - 2023.12
41	胡淑贤	国家自然科学基金委员会	面上项目	辐照下氧化铀/水界面表面腐蚀机理的量子化学研究	2020.01 - 2023.12
42	刘海广	国家自然科学基金委员会	面上项目	应用时间分辨串行晶体衍射和分子动力学模拟方法研究氯离子输运视紫 质蛋白结构和动力学	2020.01 - 2023.12
43	王冀鲁	国家自然科学基金委员会	面上项目	粘性浅水波方程的高精度数值方法	2021.01 - 2024.12
44	康　俊	国家自然科学基金委员会	面上项目	摩尔超晶格平带产生与调控机制的大规模第一性原理研究	2021.01 - 2024.12
45	李　勇	国家自然科学基金委员会	面上项目	基于量子光学方法的手性分子检测、分离与转化研究	2021.01 - 2024.12
46	任志勇	国家自然科学基金委员会	面上项目	纳米光电器件的时域模拟方法的发展与应用	2021.01 - 2024.12
47	Martin Stynes	国家自然科学基金委员会	面上项目	分数阶导数问题□-鲁棒性数值方法构造与分析	2022.01 - 2025.12
48	王艳莉	国家自然科学基金委员会	面上项目	基于玻尔兹曼方程的正则化13矩模型约简与数值模拟	2022.01 - 2025.12
49	胡时杰	国家自然科学基金委员会	面上项目	三角晶格材料中自旋液体态的大规模数值研究	2022.01 - 2025.12
50	袁凡奇	国家自然科学基金委员会	面上项目	二维超导体中的有限动量库珀对以及在摩尔超晶格中的应用	2022.01 - 2025.12
51	张　燮	国家自然科学基金委员会	面上项目	基于载流子复合机制的新型深紫外发光材料的计算设计	2022.01 - 2025.12
52	莫崇杰	国家自然科学基金委员会	理论物理专款	温稠密物质中X射线汤姆逊散射谱第一性原理计算方法的研究	2020.01 - 2020.12
53	叶　冲	国家自然科学基金委员会	理论物理专款	手性对映体测定、对映体分离和对映体转化的光学方法研究	2020.01 - 2020.12

续表

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
54	刘　磊	国家自然科学基金委员会	理论物理专款	基于非线性傅里叶变换研究光纤通信中的两类可积非线性薛定谔方程	2020.01 - 2020.12
55	胡高科	国家自然科学基金委员会	理论物理专款	非周期性边界系统的有限尺度标度理论	2020.01 - 2020.12
56	刘玉海	国家自然科学基金委员会	理论物理专款	单尺度解禁闭量子临界性及相关物理的数值研究	2020.01 - 2020.12
57	牟映坪	国家自然科学基金委员会	理论物理专款	拓扑非平庸平带系统的超导电性	2021.01 - 2021.12
58	乔　爽	国家自然科学基金委员会	理论物理专款	温度效应对于宽禁带半导体缺陷性质影响与调控的理论研究	2021.01 - 2021.12
59	崔石峰	国家自然科学基金委员会	理论物理专款	自旋为1的Spin-Peierls模型的量子相变研究	2021.01 - 2021.12
60	刘士炜	国家自然科学基金委员会	理论物理专款	强激光场中原子多重电离的电子再碰撞动力学研究	2021.01 - 2021.12
61	程　颂	国家自然科学基金委员会	理论物理专款	量子可积自旋梯子模型视角下的自旋激发与量子关联	2021.01 - 2021.12
62	胡淑贤	国家自然科学基金委员会	青年科学基金项目	含氮冠醚三价次锕系离子和镧系离子配合物成键及电子结构的理论研究	2018.01 - 2020.12
63	李　晓	国家自然科学基金委员会	青年科学基金项目	非局部相场方程的保持能量稳定与最大模稳定的高效数值方法	2019.01 - 2021.12
64	李　季	国家自然科学基金委员会	青年科学基金项目	基于矩阵分解的相位恢复非凸优化算法研究	2019.01 - 2021.12
65	陈　虎	国家自然科学基金委员会	青年科学基金项目	无界域上分数阶和非局部扩散方程的高精度数值方法研究	2019.01 - 2021.12
66	晋力京	国家自然科学基金委员会	青年科学基金项目	多模光力超导电路中非线性效应的增强和探测	2019.01 - 2021.12
67	罗智煌	国家自然科学基金委员会	青年科学基金项目	利用核自旋系统进行拓扑相量子模拟的实验研究	2019.01 - 2021.12

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
68	庞国飞	国家自然科学基金委员会	青年科学基金项目	分数阶导数对流-弥散方程参数识别的多重精度高斯过程回归算法	2018.01 - 2020.12
69	胡　麟	国家自然科学基金委员会	青年科学基金项目	非平衡态下二维宽带隙半导体中缺陷和掺杂性质的研究和调控	2018.01 - 2020.12
70	袁少杰	国家自然科学基金委员会	青年科学基金项目	超导量子比特的弱测量及其量子力学时间对称性的研究	2018.01 - 2020.12
71	康　雷	国家自然科学基金委员会	青年科学基金项目	典型狄拉克材料的非线性光学性质的理论研究	2018.01 - 2020.12
72	张春芳	国家自然科学基金委员会	青年科学基金项目	芳香烃超导材料制备中涉及的化学反应的理论研究	2018.01 - 2020.12
73	吴　威	国家自然科学基金委员会	青年科学基金项目	量子开放系统动力学的数值研究	2018.01 - 2020.12
74	张闻钊	国家自然科学基金委员会	青年科学基金项目	开放量子系统中光机械振子辐射压冷却的理论研究	2018.01 - 2020.12
75	黄卫杰	国家自然科学基金委员会	青年科学基金项目	表面扩散流的保结构高效数值算法	2021.01 - 2023.12
76	郭震林	国家自然科学基金委员会	青年科学基金项目	带表面活性剂的两相流相场模型建模与数值求解	2021.01 - 2023.12
77	王建峰	国家自然科学基金委员会	青年科学基金项目	拓扑半金属的等离激元及其在太赫兹领域应用的理论研究	2021.01 - 2023.12
78	房一楠	国家自然科学基金委员会	青年科学基金项目	对称性度量在多比特量子随机基准中的应用	2021.01 - 2023.12
79	莫崇杰	国家自然科学基金委员会	青年科学基金项目	温稠密物质X射线光谱的第一性原理研究	2021.01 - 2023.12
80	孙庆德	国家自然科学基金委员会	青年科学基金项目	高光吸收材料的物理机理研究	2021.01 - 2023.12
81	贾略羚	国家自然科学基金委员会	青年科学基金项目	三维稀疏谱方法及其快速算法的研究	2022.01 - 2024.12

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No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
82	王丽修	国家自然科学基金委员会	青年科学基金项目	四阶旋度电磁场方程协调谱元方法的设计、理论及应用	2022.01 - 2024.12
83	周永涛	国家自然科学基金委员会	青年科学基金项目	带弱奇异核的Volterra积分和积分-微分方程的块边值方法研究	2022.01 - 2024.12
84	贾甜甜	国家自然科学基金委员会	青年科学基金项目	利用电子轨道杂化理论探索良好热电材料中强非简谐效应的本质来源	2022.01 - 2024.12
85	肖　磊	国家自然科学基金委员会	青年科学基金项目	宇称-时间对称系统中临界点性质及应用的实验研究	2022.01 - 2024.12
86	童　贞	国家自然科学基金委员会	青年科学基金项目	低维材料中位错缺陷热输运特性的原子尺度模拟	2022.01 - 2024.12
87	Jorge Botana Alcalde	国家自然科学基金委员会	外国青年学者基金项目	Design of mixed-anion structures for industrial applications	2019.01 - 2020.12
88	Rubem Mondaini	国家自然科学基金委员会	外国青年学者基金项目	Out-of-equilibrium systems: Thermalization, Many-body localization and topological Time-crystals	2019.01 - 2020.12
89	Georg Engelhardt	国家自然科学基金委员会	外国青年学者基金项目	Spectroscopy of molecular excitation dynamics- far beyond linear response	2020.01 - 2020.12
90	Rubem Mondaini	国家自然科学基金委员会	外国青年学者基金项目	Giant magnetoresistance and correlated physics in twisted bilayer graphene: large scale numerical study using quantum-classical Hamiltonians	2021.01 - 2022.12
91	冼　殷	中国博士后科学基金	博士后国际交流计划引进项目	—	2018.10 - 2020.09
92	Georg Engelhardt	中国博士后科学基金	博士后国际交流计划引进项目	—	2018.10 - 2020.09
93	马小磊	中国博士后科学基金	博士后国际交流计划引进项目	—	2019.06 - 2021.05
94	杨雪清	中国博士后科学基金	博士后国际交流计划引进项目	—	2019.11 - 2021.10

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
95	黄卫杰	中国博士后科学基金	博士后国际交流计划派出项目	—	2019.07 - 2021.06
96	景晓波	中国博士后科学基金	博士后国际交流计划派出项目	—	2019.07 - 2021.06
97	李　培	中国博士后科学基金	博士后国际交流计划派出项目	—	2021.07 - 2023.07
98	马小磊	中国博士后科学基金	特别资助（站前）	关于active matter中压强的研究	2019.06 - 2021.05
99	徐小绪	中国博士后科学基金	特别资助（站前）	无相位反散射问题的唯一性和数值算法	2019.06 - 2021.05
100	陶　琪	中国博士后科学基金	特别资助（站前）	求解空间高阶导数方程超弱局部间断有限元方法的误差估计及超收敛研究	2020.08 - 2022.07
101	刘玉海	中国博士后科学基金	特别资助（站中）	自发对称破缺量子自旋霍尔态相关物理问题的数值研究	2020.08 - 2022.07
102	莫崇杰	中国博士后科学基金	特别资助（站中）	温稠密物质X射线光谱的第一性原理方法研究	2020.08 - 2022.07
103	肖　磊	中国博士后科学基金	特别资助（站中）	光量子行走中非布洛赫宇称-时间对称破缺的实验研究	2021.06 - 2023.06
104	王　威	中国博士后科学基金	面上一等资助	特征值问题的大规模、高精度快速算法研究	2018.12 - 2020.11
105	Georg Engelhardt	中国博士后科学基金	面上一等资助	开放量子系统的调控	2018.12 - 2020.11
106	张煜然	中国博士后科学基金	面上一等资助	量子拓扑态的多体纠缠性质的研究	2018.12 - 2020.11
107	王坤坤	中国博士后科学基金	面上一等资助	非厄米系统中Leggett-Gary不等式的实验研究	2019.11 - 2021.10
108	莫崇杰	中国博士后科学基金	面上一等资助	温稠密物质中X射线汤姆逊散射谱的理论模拟研究	2019.11 - 2021.10

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No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
109	肖　磊	中国博士后科学基金	面上一等资助	光量子行走中拓扑性质的实验研究	2020.11 - 2022.10
110	赵腾飞	中国博士后科学基金	面上二等资助	关于外域上非线性Schrodinger方程的数学研究	2019.05 - 2021.04
111	Ben Aicha Ibtissem	中国博士后科学基金	面上二等资助	单组测量数据的时域反问题的唯一性和稳定性	2019.05 - 2021.04
112	陈　升	中国博士后科学基金	面上二等资助	几类奇异摄动问题的高精度谱/谱元法	2019.05 - 2021.04
113	宫　博	中国博士后科学基金	面上二等资助	求解一类带有模式转换的随机最优控制问题的数值方法	2019.05 - 2021.04
114	Pankaj Bhalla	中国博士后科学基金	面上二等资助	拓扑量子物质中的信息传递	2019.05 - 2021.04
115	李珍珍	中国博士后科学基金	面上二等资助	表面吸附模型中自旋声子耦合作用的研究	2019.05 - 2021.04
116	邵　灿	中国博士后科学基金	面上二等资助	低维强关联系统的非平衡超快动力学研究	2019.05 - 2021.04
117	刘　磊	中国博士后科学基金	面上二等资助	运用非线性傅里叶变换分析和计算光纤脉冲的演化和调制	2019.11 - 2021.10
118	程永喜	中国博士后科学基金	面上二等资助	多轨道杂质系统中多体效应依赖的热电输运特性	2019.11 - 2021.10
119	刘玉海	中国博士后科学基金	面上二等资助	拓展的Kane-Mele模型的深入数值研究	2019.11 - 2021.10
120	王云华	中国博士后科学基金	面上二等资助	二维材料中压电铁电效应和关联效应的理论研究	2019.11 - 2021.10
121	洪　旗	中国博士后科学基金	面上二等资助	复杂流体相场模型高效、高精度保结构算法的研究与应用	2020.07 - 2022.06
122	王丽修	中国博士后科学基金	面上二等资助	H（curl^2）协调谱元的构造及其应用	2020.07 - 2022.06

No.	项目负责人 PI	经费来源 SOURCE	项目类别 CATEGORY	项目名称 PROJECT TITLE	起止时间 FROM AND TO
123	鲁少华	中国博士后科学基金	面上二等资助	新型碳/硅基二维催化材料的理论设计	2020.07 - 2022.06
124	韩家宇	中国博士后科学基金	面上二等资助	Maxwell传输特征值问题的高效数值方法	2020.11 - 2022.10
125	李　刚	中国博士后科学基金	面上二等资助	基于弱测量的光力学系统中非线性放大作用和量子精密测量的研究	2020.11 - 2022.10
126	王文元	中国博士后科学基金	面上二等资助	自旋轨道耦合玻色-爱因斯坦凝聚体的非线性量子相干调控	2020.11 - 2022.10
127	李　培	中国博士后科学基金	面上二等资助	无序/有序界面缺陷的物理性质及调控方法的研究	2020.11 - 2022.10
128	周永涛	中国博士后科学基金	面上二等资助	带弱奇异核Volterra型方程的分层网格块边值方法	2021.06 - 2023.06
129	刘　博	中国博士后科学基金	面上二等资助	对称陀螺型手性分子的探测、分离和转化	2021.06 - 2023.06
130	陈元正	中国博士后科学基金	面上二等资助	探究二元二维 II-P 磷化物结构中元素电负性差异对磷“孤对电子”键调控作用和结构有氧环境稳定性影响	2021.06 - 2023.06
131	赫龄君	中国博士后科学基金	面上二等资助	稀土掺杂全无机钙钛矿材料的物性研究	2021.06 - 2023.06
132	贾甜甜	中国博士后科学基金	面上二等资助	Pyrite型热电材料中强非简谐效应的物理机制探索	2021.06 - 2023.06
133	聂运欢	中国博士后科学基金	面上二等资助	二维软芯系统超晶格相形成规律及其振动特性研究	2021.06 - 2023.06
134	乔　爽	中国博士后科学基金	面上二等资助	温度效应对于宽禁带半导体缺陷性质影响与调控的理论研究	2021.06 - 2023.06
135	苏　威	中国博士后科学基金	面上二等资助	SU（4）格子模型中拓扑液体态的大规模数值研究	2021.06 - 2023.06

2020-2021学术年期间，中心合计发表论文约371篇，其中归属中心（包括第一单位及通讯作者第一单位）论文205篇，其他合作论文166篇。

During the 2020-2021 academic year, CSRC has published a total of about 371 papers.

SIMULATION OF PHYSICAL SYSTEMS DIVISION 物理系统模拟研究部

1	Observation of energy-resolved many-body localization; Guo, Qiujiang; Cheng, Chen; Sun, Zheng-Hang; Song, Zixuan; Li, Hekang; Wang, Zhen; Ren, Wenhui; Dong, Hang; Zheng, Dongning; Zhang, Yu-Ran; Mondaini, Rubem; Fan, Heng; Wang, H.; NATURE PHYSICS, 17, 2 (2021)
2	Asymmetric Light Scattering on Heterodimers Made of Au Nanorods Vertically Standing on Au Nanodisks; Lai, Yunhe; Cui, Ximin; Li, Nannan; Shao, Lei; Zhang, Wei; Wang, Jianfang; Lin, Hai-Qing; ADVANCED OPTICAL MATERIALS, 9, 3 (2021)
3	Electrophoretic Plasmonic Ink for Dynamic Color Display; Zheng, Jiapeng; Chow, Tsz Him; Li, Shasha; Wang, Jianfang; Shao, Lei; ADVANCED OPTICAL MATERIALS, 9, 12 (2021)
4	Emergence and Disruption of Spin-Charge Separation in One-Dimensional Repulsive Fermions; He, Feng; Jiang, Yu-Zhu; Lin, Hai-Qing; Hulet, Randall G.; Pu, Han; Guan, Xi-Wen; PHYSICAL REVIEW LETTERS, 125, 19 (2020)
5	(Gold nanorod core)/(poly(3,4-ethylene-dioxythiophene) shell) nanostructures and their monolayer arrays for plasmonic switching; Liang, Lili; Lam, Shiu Hei; Ma, Lijuan; Lu, Wenzheng; Wang, Shi-Bin; Chen, Aizheng; Wang, Jianfang; Shao, Lei; Jiang, Nina; NANOSCALE, 12, 40 (2020)
6	Strain gradient induced spatially indirect excitons in single crystalline ZnO nanowires; Liu, Zhao; Fu, Xuewen; Zhang, Dong-Bo; NANOSCALE, 12, 37 (2020)
7	Control of light-valley interactions in 2D transition metal dichalcogenides with nanophotonic structures; Li, Shasha; Wang, Hao; Wang, Jing; Chen, Huanjun; Shao, Lei; NANOSCALE, 13, 13 (2021)
8	Chirality-selective transparency induced by lattice resonance in bilayer metasurfaces; Zhao, Shuxia; Shao, Lei; Wang, Jianfang; Lin, Hai-Qing; Zhang, Wei; PHOTONICS RESEARCH, 9, 4 (2021)
9	Electrically pumped terahertz laser based on a topological insulator quantum dot array; Huang, YongWei; Shi, Likun; Li, Jun; Lou, WenKai; Yuan, HuiHong; Yang, Wen; Chang, Kai; SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY, 64, 1 (2021)
10	Novel Two-Dimensional Layered MoSi(2)Z(4) (Z = P, As): New Promising Optoelectronic Materials; Yao, Hui; Zhang, Chao; Wang, Qiang; Li, Jianwei; Yu, Yunjin; Xu, Fuming; Wang, Bin; Wei, Yadong; NANOMATERIALS, 11, 3 (2021)

11	Learning Order Parameters from Videos of Skyrmion Dynamical Phases with Neural Networks; Wang, Weidi; Wang, Zeyuan; Zhang, Yinghui; Sun, Bo; Xia, Ke; PHYSICAL REVIEW APPLIED, 16, 1 (2021)
12	Balancing coherent and dissipative dynamics in a central-spin system; Ricottone, A.; Fang, Y. N.; Coish, W. A.; PHYSICAL REVIEW B, 102, 8 (2020)
13	First-principles method for x-ray Thomson scattering including both elastic and inelastic features in warm dense matter; Mo, Chongjie; Fu, Zhen-Guo; Zhang, Ping; Kang, Wei; Zhang, Weiyan; He, X. T.; PHYSICAL REVIEW B, 102, 19 (2020)
14	First-principles study of solid hydrogen: Comparison among four exchange-correlation functionals; Yang, Huan-Cheng; Liu, Kai; Lu, Zhong-Yi; Lin, Hai-Qing; PHYSICAL REVIEW B, 102, 17 (2020)
15	Magnetoresistance effects in a spin-fermion model for multilayers; Tarat, Sabyasachi; Li, Jian; Scalettar, Richard T.; Mondaini, Rubem; PHYSICAL REVIEW B, 102, 9 (2020)
16	Nonequilibrium phases and phase transitions of the XY model; Puel, Tharnier O.; Chesi, Stefano; Kirchner, Stefan; Ribeiro, Pedro; PHYSICAL REVIEW B, 103, 3 (2021)
17	Interplay of local order and topology in the extended Haldane-Hubbard model; Shao, Can; Castro, Eduardo, V; Hu, Shijie; Mondaini, Rubem; PHYSICAL REVIEW B, 103, 3 (2021)
18	First-principles study of the anomalous Hall effect based on exact muffin-tin orbitals; Wang, Lei; Min, Tai; Xia, Ke; PHYSICAL REVIEW B, 103, 5 (2021)
19	Intrinsic contribution to nonlinear thermoelectric effects in topological insulators; Bhalla, Pankaj; PHYSICAL REVIEW B, 103, 11 (2021)
20	Superradiantlike dynamics of nuclear spins by nonadiabatic electron shuttling; Fang, Yinan; Wang, Ying-Dan; Fazio, Rosario; Chesi, Stefano; PHYSICAL REVIEW B, 103, 15 (2021)
21	Robust wavefront dislocations of Friedel oscillations in gapped graphene; Zhang, Shu-Hui; Yang, Jin; Shao, Ding-Fu; Wu, Zhenhua; Yang, Wen; PHYSICAL REVIEW B, 103, 16 (2021)
22	Friedel oscillations in graphene gapped by breaking P and T symmetries: Topological and geometrical signatures of electronic structure; Yang, Jin; Shao, Ding-Fu; Zhang, Shu-Hui; Yang, Wen; PHYSICAL REVIEW B, 104, 3 (2021)
23	Gross-Neveu Heisenberg criticality: Dynamical generation of quantum spin Hall masses; Liu, Yuhai; Wang, Zhenjiu; Sato, Toshihiro; Guo, Wenan; Assaad, Fakher F.; PHYSICAL REVIEW B, 104, 3 (2021)
24	Time crystals in the driven transverse field Ising model under quasiperiodic modulation; Liang, Pengfei; Fazio, Rosario; Chesi, Stefano; NEW JOURNAL OF PHYSICS, 22, 12 (2020)

SIMULATION OF PHYSICAL SYSTEMS DIVISION 物理系统模拟研究部

25	Structures, electronic properties, and superconductivities of alkaline-earth metal-doped phenanthrene and charge transfer characteristics of metal-doped phenanthrene; Gao, Lei; Zhong, Guo-Hua; Lin, Hai-Qing; PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 22, 41 (2020)
26	Fluid Meniscus Algorithms for Dynamic Pore-Network Modeling of Immiscible Two-Phase Flow in Porous Media; Sinha, Santanu; Gjennestad, Magnus Aa.; Vassvik, Morten; Hansen, Alex; FRONTIERS IN PHYSICS, 8 (2021)
27	Crack localization and the interplay between stress enhancement and thermal noise; Sinha, Santanu; Roy, Subhadeep; Hansen, Alex; PHYSICA A-STATISTICAL MECHANICS AND ITS APPLICATIONS, 569 (2021)
28	Linear combination estimator of multiple-outcome detections with discrete measurement outcomes; Zhou, L. K.; Xu, J. H.; Zhang, W-Z; Cheng, J.; Yin, T. S.; Yu, Y. B.; Chen, R. P.; Chen, A. X.; Jin, G. R.; Yang, W.; PHYSICAL REVIEW A, 103, 4 (2021)
29	Lower and upper bounds of quantum battery power in multiple central spin systems; Peng, Li; He, Wen-Bin; Chesi, Stefano; Lin, Hai-Qing; Guan, Xi-Wen; PHYSICAL REVIEW A, 103, 5 (2021)
30	Molecular dynamics investigation of the stopping power of warm dense hydrogen for electrons; Liu, Yun; Liu, Xing; Zhang, Shen; Liu, Hao; Mo, Chongjie; Fu, Zhenguo; Dai, Jiayu; PHYSICAL REVIEW E, 103, 6 (2021)
31	Optical phonon contribution to the thermal conductivity of a quantum paraelectric; Bhalla, Pankaj; Das, Nabyendu; JOURNAL OF PHYSICS-CONDENSED MATTER, 33, 34 (2021)
32	Quantum phase transitions and critical behaviors in the two-mode three-level quantum Rabi model; Zhang, Yan; Mao, Bin-Bin; Xu, Dazhi; Zhang, Yu-Yu; You, Wen-Long; Liu, Maoxin; Luo, Hong-Gang; JOURNAL OF PHYSICS A-MATHEMATICAL AND THEORETICAL, 53, 31 (2020)
33	Phase transitions and correlations in fracture processes where disorder and stress compete; Sinha, Santanu; Roy, Subhadeep; Hansen, Alex; PHYSICAL REVIEW RESEARCH, 2, 4 (2020)
34	Unusual excitations and double-peak specific heat in a bond-alternating spin-1 K-Gamma chain; Luo, Qiang; Hu, Shijie; Kee, Hae-Young; PHYSICAL REVIEW RESEARCH, 3, 3 (2021)

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9	Second order linear decoupled energy dissipation rate preserving schemes for the Cahn-Hilliard-extended-Darcy model; Yakun Li;Wenkai Yu;Jia Zhao;Qi Wang; JOURNAL OF COMPUTATIONAL PHYSICS, 444 (2021)
10	A discrete comparison principle for the time-fractional diffusion equation; Chen, Hu; Stynes, Martin; COMPUTERS & MATHEMATICS WITH APPLICATIONS, 80, 5 (2020)
11	A locking-free weak Galerkin finite element method for Reissner-Mindlin plate on polygonal meshes; Ye, Xiu; Zhang, Shangyou; Zhang, Zhimin; COMPUTERS & MATHEMATICS WITH APPLICATIONS, 80, 5 (2020)
12	Seven-velocity three-dimensional vectorial lattice Boltzmann method including various types of approximations to the pressure and two-parameterized second-order boundary treatments; Zhao, Jin; Zhang, Zhimin; COMPUTERS & MATHEMATICS WITH APPLICATIONS, 80, 12 (2020)
13	Energy-production-rate preserving numerical approximations to network generating partial differential equations; Hong, Qi; Zhao, Jia; Wang, Qi; COMPUTERS & MATHEMATICS WITH APPLICATIONS, 84 (2021)
14	A Hodge Decomposition Method for Dynamic Ginzburg-Landau Equations in Nonsmooth Domains - A Second Approach; Li, Buyang; Wang, Kai; Zhang, Zhimin; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 28, 2 (2020)
15	Multi-Scale Deep Neural Network (MscaleDNN) for Solving Poisson-Boltzmann Equation in Complex Domains; Liu, Ziqi; Cai, Wei; Xu, Zhi-Qin John; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 28, 5 (2020)
16	Discrete-Velocity Vector-BGK Models Based Numerical Methods for the Incompressible Navier-Stokes Equations; Zhao, Jin; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 29, 2 (2021)
17	A Mortar Spectral Element Method for Full-Potential Electronic Structure Calculations; Guo, Yichen; Jia, Lueling; Chen, Huajie; Li, Huiyuan; Zhang, Zhimin; COMMUNICATIONS IN COMPUTATIONAL PHYSICS, 29, 5 (2021)
18	CONVERGENCE OF A SECOND-ORDER ENERGY-DECAYING METHOD FOR THE VISCOUS ROTATING SHALLOW WATER EQUATION; Akrivis, Georgios; Li, Buyang; Wang, Jilu; SIAM JOURNAL ON NUMERICAL ANALYSIS, 59, 1 (2021)
19	Fast evaluation of artificial boundary conditions for advection diffusion equations; Sun, Ting; Wang Jilu; Zheng, Chunxiong; SIAM JOURNAL ON NUMERICAL ANALYSIS, 58 (2020)

APPLIED AND COMPUTATIONAL MATHEMATICS DIVISION 应用与计算数学研究部

20	Barycentric prolate interpolation and pseudospectral differentiation; Tian, Yan; NUMERICAL ALGORITHMS, (2021)
21	Rogue waves of ultra-high peak amplitude: a mechanism for reaching up to a thousand times the background level; Sun, Wen-Rong; Liu, Lei; Kevrekidis, P. G.; PROCEEDINGS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES, 477, 2246 (2021)
22	Energy-stable predictor-corrector schemes for the Cahn-Hilliard equation; Zhang, Jun; Jiang, Maosheng; Gong, Yuezheng; Zhao, Jia; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 376 (2020)
23	A finite difference method for an initial-boundary value problem with a Riemann-Liouville-Caputo spatial fractional derivative; Luis Gracia, Jose; Stynes, Martin; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 381 (2021)
24	An alpha-robust finite element method for a multi-term time-fractional diffusion problem; Huang, Chaobao; Stynes, Martin; Chen, Hu; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 389 (2021)
25	Sharp H-1-norm error estimates of two time-stepping schemes for reaction-subdiffusion problems; Ren, Jincheng; Liao, Hong-lin; Zhang, Jiwei; Zhang, Zhimin; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 389 (2021)
26	A CG-DG method for Maxwell's equations in Cole–Cole dispersive media; Wang, Jiangxing; Zhang, Jiwei; and Zhang, Zhimin; JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS, 393 (2021)
27	Blow-up of error estimates in time-fractional initial-boundary value problems; Chen, Hu; Stynes, Martin; IMA JOURNAL OF NUMERICAL ANALYSIS, 41, 2 (2021)
28	Superconvergence Error Estimate of a Finite Element Method on Nonuniform Time Meshes for Reaction-Subdiffusion Equations; Ren, Jincheng; Liao, Hong-lin; Zhang, Zhimin; JOURNAL OF SCIENTIFIC COMPUTING, 84, 2 (2020)
29	An alpha-Robust Semidiscrete Finite Element Method for a Fokker-Planck Initial-Boundary Value Problem with Variable-Order Fractional Time Derivative; Le, Kim-Ngan; Stynes, Martin; JOURNAL OF SCIENTIFIC COMPUTING, 86, 2 (2021)
30	A Single-Step Correction Scheme of Crank-Nicolson Convolution Quadrature for the Subdiffusion Equation; Wang, Jilu; Wang, Jungang; Yin, Lihong; JOURNAL OF SCIENTIFIC COMPUTING, 87, 1 (2021)
31	Finite Element Calculation of Photonic Band Structures for Frequency Dependent Materials; Xiao, Wenqiang; Gong, Bo; Sun, Jiguang; Zhang, Zhimin; JOURNAL OF SCIENTIFIC COMPUTING, 87, 1 (2021)
32	Scalable Incremental Nonconvex Optimization Approach for Phase Retrieval; Li, Ji; Cai, Lian-Feng; Zhao, Hongkai; JOURNAL OF SCIENTIFIC COMPUTING, 87, 2 (2021)
33	A Rational Approximation Scheme for Computing Mittag-Leffler Function with Discrete Elliptic Operator as Input; Duan, Beiping; Zhang, Zhimin; JOURNAL OF SCIENTIFIC COMPUTING, 87, 3 (2021)

34	Thermodynamically Consistent Algorithms for Models of Diblock Copolymer Solutions Interacting with Electric and Magnetic Fields; Shen, Xiaowen; Wang, Qi; JOURNAL OF SCIENTIFIC COMPUTING, 88, 43 (2021)
35	Implicit-explicit time integration of nonlinear fractional differential equations; Zhou, Yongtao; Suzuki, Jorge L.; Zhang, Chengjian; Zayernouri, Mohsen; APPLIED NUMERICAL MATHEMATICS, 156 (2020)
36	Numerical analysis on the mortar spectral element methods for Schrodinger eigenvalue problem with an inverse square potential; Jia, Lueling; Li, Huiyuan; Zhang, Zhimin; APPLIED NUMERICAL MATHEMATICS, 158 (2020)
37	ANALYSIS OF ADAPTIVE BDF2 SCHEME FOR DIFFUSION EQUATIONS; Liao, Hong-lin; Zhang, Zhimin; MATHEMATICS OF COMPUTATION, 90, 329 (2021)
38	Uniqueness to inverse acoustic scattering from coated polygonal obstacles with a single incoming wave; Hu, Guang-Hui; Vashisth, Manmohan; INVERSE PROBLEMS, 36, 10 (2020)
39	A spectrally accurate approximation to subdiffusion equations using the log orthogonal functions; Chen, Sheng; Shen, Jie; Zhang, Zhimin; and Zhou, Zhi; SIAM JOURNAL ON SCIENTIFIC COMPUTING, 42, 2 (2020)
40	Vector-type boundary schemes for the lattice Boltzmann method based on vector-BGK models; Zhao, Jin; Zhang, Zhimin; and Yong, Wen-An; SIAM JOURNAL ON SCIENTIFIC COMPUTING, 42, 5 (2020)
41	Central vortex steady states and dynamics of Bose-Einstein condensates interacting with a microwave field; Wang, Di; Cai, Yongyong; Wang, Qi; PHYSICA D-NONLINEAR PHENOMENA, 419 (2021)
42	A weighted and balanced FEM for singularly perturbed reaction-diffusion problems; Madden, Niall; Stynes, Martin; CALCOLO, 58, 2 (2021)
43	Band structure calculation of photonic crystals with frequency-dependent permittivities; XIAO, W. E. N. Q. I. A. N. G.; SUN, J. I. G. U. A. N. G.; JOURNAL OF THE OPTICAL SOCIETY OF AMERICA A-OPTICS IMAGE SCIENCE AND VISION, 38, 5 (2021)
44	A recovery-based linear C-0 finite element method for a fourth-order singularly perturbed Monge-Ampere equation; Chen, Hongtao; Feng, Xiaobing; Zhang, Zhimin; ADVANCES IN COMPUTATIONAL MATHEMATICS, 47, 2 (2021)
45	Block boundary value methods for linear weakly singular Volterra integro-differential equations; Zhou, Yongtao; Stynes, Martin; BIT NUMERICAL MATHEMATICS, 61, 2 (2021)
46	A priori error estimates of discontinuous Galerkin methods for a quasi-variational inequality; Wang, Fei; Shah, Sheheryar; Xiao, Wenqiang; BIT NUMERICAL MATHEMATICS, (2021)
47	An Alternative Finite Difference Stability Analysis for a Multiterm Time-Fractional Initial-Boundary Value Problem; Liu, Xiaohui; Stynes, Martin; EAST ASIAN JOURNAL ON APPLIED MATHEMATICS, 10, 3 (2020)

APPLIED AND COMPUTATIONAL MATHEMATICS DIVISION 应用与计算数学研究部

48	A theta-L Formulation-Based Finite Element Method for Solving Axisymmetric Solid-State Dewetting Problems; Huang, Weijie; Jiang, Wei; Zhao, Quan; EAST ASIAN JOURNAL ON APPLIED MATHEMATICS, 11, 2 (2021)
49	Uniqueness for time-dependent inverse problems with single dynamical data; Ben Aicha, Ibtissem; Hu, Guang-Hui; Vashisth, Manmohan; Zou, Jun; JOURNAL OF MATHEMATICAL ANALYSIS AND APPLICATIONS, 497, 2 (2021)
50	Error Analysis of a Finite Difference Method on Graded Meshes for a Multiterm Time-Fractional Initial-Boundary Value Problem; Huang, Chaobao; Liu, Xiaohui; Meng, Xiangyun; Stynes, Martin; COMPUTATIONAL METHODS IN APPLIED MATHEMATICS, 20, 4 (2020)
51	A C-1 PETROV-GALERKIN METHOD AND GAUSS COLLOCATION METHOD FOR 1D GENERAL ELLIPTIC PROBLEMS AND SUPERCONVERGENCE; Cao, Waixiang; Jia, Lueling; Zhang, Zhimin; DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS-SERIES B, 26, 1 (2021)
52	APPROXIMATION METHODS FOR THE DISTRIBUTED ORDER CALCULUS USING THE CONVOLUTION QUADRATURE; Yin, Baoli; Liu, Yang; Li, Hong; Zhang, Zhimin; DISCRETE AND CONTINUOUS DYNAMICAL SYSTEMS-SERIES B, 26, 3 (2021)
53	MODERATE MAXIMAL INEQUALITIES FOR THE ORNSTEIN-UHLENBECK PROCESS; Jia, Chen; Zhao, Guohuan; PROCEEDINGS OF THE AMERICAN MATHEMATICAL SOCIETY, 148, 8 (2020)
54	Uniqueness in inverse electromagnetic scattering problem with phaseless far-field data at a fixed frequency; Xu, Xiaoxu; Zhang, Bo; Zhang, Haiwen; IMA JOURNAL OF APPLIED MATHEMATICS, 85, 6 (2020)
55	A family of curl-curl conforming finite elements on tetrahedral meshes; Zhang, Qian; and Zhang Zhimin; CSIAM Transactions on Applied Mathematics, 1, 4 (2020)

MECHANICS DIVISION 力学研究部

1	Roads to Smart Artificial Microswimmers; Tsang, Alan C. H.; Demir, Ebru; Ding, Yang; Pak, On Shun; ADVANCED INTELLIGENT SYSTEMS, 2, 8 (2020)
2	A diffuse domain method for two-phase flows with large density ratio in complex geometries; Guo, Zhenlin; Yu, Fei; Lin, Ping; Wise, Steven; Lowengrub, John; JOURNAL OF FLUID MECHANICS, 907 (2021)
3	Hermite spectral method for Fokker-Planck-Landau equation modeling collisional plasma; Li, Ruo; Ren, Yinuo; Wang, Yanli; JOURNAL OF COMPUTATIONAL PHYSICS, 434 (2021)
4	Swimming of the mosquito larva: principles and tricks of locomotion at intermediate Reynolds numbers; Jin, B.; Luo, H.; Ding, Y.; INTEGRATIVE AND COMPARATIVE BIOLOGY, 61 (2021)

MECHANICS DIVISION 力学研究部

5	Stokes Eigenmodes on two-dimensional regular polygons; Pierre Lallemanda; Lizhen Chen; Gérard Labrosseab; Li–Shi Luo; Computers & Fluids, 228, 15 (2021)
6	Nonlocal shear-thinning effects substantially enhance helical propulsion; Demir, Ebru; Lordi, Noah; Ding, Yang; Pak, On Shun; PHYSICAL REVIEW FLUIDS, 5, 11 (2020)
7	Base flow decomposition for complex moving objects in linear hydrodynamics: Application to helix-shaped flagellated microswimmers; Zhang, Ji; Chinappi, Mauro; Biferale, Luca; PHYSICAL REVIEW E, 103, 2 (2021)
8	Direct numerical study of speed of sound in dispersed air-water two-phase flow; Fu, Kai; Deng, Xiaolong; Jiang, Lingjie; Wang, Pengfei; WAVE MOTION, 98 (2020)
9	Tail shapes lead to different propulsive mechanisms in the body/caudal fin undulation of fish; Song, Jialei; Zhong, Yong; Du, Ruxu; Yin, Ling; Ding, Yang; PROCEEDINGS OF THE INSTITUTION OF MECHANICAL ENGINEERS PART C-JOURNAL OF MECHANICAL ENGINEERING SCIENCE, 235, 2 (2021)

ALGORITHMS DIVISION 计算方法研究部

1	Electric Field Tunable Ultrafast Interlayer Charge Transfer in Graphene/WS2 Heterostructure; Liu, Yuxiang; Zhang, Jin; Meng, Sheng; Yam, ChiYung; Frauenheim, Thomas; NANO LETTERS, 21, 10 (2021)
2	Photoinduced charge-transfer in chromophore-labeled gold nanoclusters: quantum evidence of the critical role of ligands and vibronic couplings; Dominguez-Castro, Adrian; Lien-Medrano, Carlos R.; Maghrebi, Khaoula; Messaoudi, Sabri; Frauenheim, Thomas; Fihey, Arnaud; NANOSCALE, 13, 14 (2021)
3	Numerical variational solution of hydrogen molecule and ions using one-dimensional hydrogen as basis functions; Sarwono, Yanoar Pribadi; Rahman, Faiz Ur; Zhang, Ruiqin; NEW JOURNAL OF PHYSICS, 22, 9 (2020)
4	A Jacobi spectral method for computing eigenvalue gaps and their distribution statistics of the fractional Schrodinger operator; Bao, Weizhu; Chen, Lizhen; Jiang, Xiaoyun; Ma, Ying; JOURNAL OF COMPUTATIONAL PHYSICS, 421 (2020)
5	A novel second-order linear scheme for the Cahn-Hilliard-Navier-Stokes equations; Chen, Lizhen; Zhao, Jia; JOURNAL OF COMPUTATIONAL PHYSICS, 423 (2020)
6	Error estimates of finite difference methods for the Dirac equation in the massless and nonrelativistic regime; Ma, Ying; Yin, Jia; NUMERICAL ALGORITHMS, (2021)
7	Solution of two-electron Schrodinger equations using a residual minimization method and one-dimensional basis functions; Rahman, Faiz Ur; Sarwono, Yanoar Pribadi; Zhang, Rui-Qin; AIP ADVANCES, 11, 2 (2021)

WORKSHOPS & CONFERENCES (2020-2021) 中心主办、合办的学术会议

时间 Date	会议名称 Title
2021.07.19-21	5th Conference on Numerical Methods for Fractional-derivative Problems 第五届分数微分问题数值方法会议
2021.07.14-19	2021 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry 2021年理论与计算物理与化学前沿国际研讨会
2021.06.28-07.10	Workshop and Summer School on Kinetic Theory and Related Applications 动力学理论及相关应用研讨会
2021.06.01-06	International CECAM-Workshop on Real-time quantum dynamics in photo-stimulated processes: experiment and theory 国际CECAM 研讨会-光刺激过程中的实时量子动力学：实验和理论
2021.05.15-16	Workshop on Numerical Methods and Analysis of Differential Equations 微分方程数值方法及分析研讨会
2021.05.08-09	International Conference on Eigenvalue Problems and Related Topics 特征值问题及相关主题国际会议
2020.12.04-07	2020 International Workshop on Frontiers of Theoretical and Computational Physics and Chemistry 2020 理论与计算物理与化学前沿国际研讨会
2020.11.6	清华大学—北京计算科学研究中心双边研讨会
2020.10.22-24	4th Conference on Numerical Methods for Fractional-derivative Problems 第四届分数微分问题数值方法会议

TUTORIALS (2020-2021) 培训班

时间 Date	会议名称 Title
2021.7.14-18	强关联体系理论与算法培训班
2021.05.03-07	电磁场问题与特征值问题的有限元方法培训班
2020.12.3-7	电子结构计算中的线性标度理论方法培训班
2020.11.9-12	材料与能源前沿科学：非平衡态物理和计算方法培训班
2020.10.25-27	量子精密测量培训班

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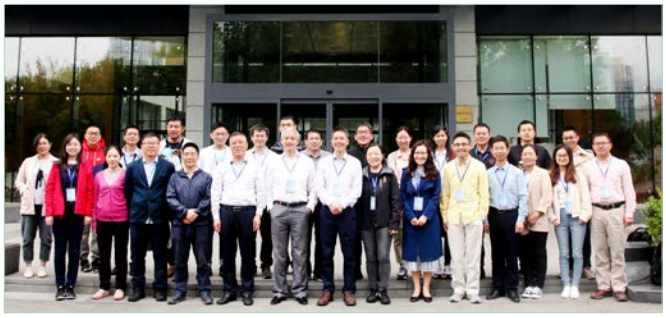

CSRC SEMINAR 专题报告

中心积极邀请国内外相关领域重要学者举行专题报告，活跃学术氛围，激发学术思维。2020-2021学术年期间中心共举办专题讲座98期（总1010期）。

CSRC invites national and overseas leading researchers to give academic seminars. During academic year 2020-2021, CSRC held 98 seminars.

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
1	2020-8-25	解西国 Xi-Guo Xie	曙光高性能计算产品事业部 HPC Product Division, Sugon	Recent Progresses in home-made HPC, Sugon
2	2020-9-9	阚二军 Er-Jun Kan	南京理工大学 Nanjing University of Science and Technology, China	铁磁性材料的理论研究 Theoretical study of ferromagnetic materials
3	2020-9-24	李杰权 Jie-Quan Li	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	The role of entropy in CFD
4	2020-9-25	张　俊 Jun Zhang	中科院半导体所 SKLSM, Institute of Semiconductors, CAS, China	Laser Cooling of Lattice Phonons in Semiconductors
5	2020-10-9	董　彬 Bin Dong	北京大学北京国际数学研究中心 Beijing International Center for Mathematical Research, Peking University	Deep CT Imaging by Unrolled Dynamics
6	2020-10-13	Suchuan Dong	普渡大学 Purdue University, USA	Open Boundaries in Two-Pahse and Multiphase Flows: Energy-Stable Open Boundary Conditions
7	2020-10-21	刘奇航 Qi-Hang Liu	南方科技大学 Southern University of Science and Technology, China	Routes to quantum anomalous Hall effect from magnetic topological insulators $MnBi_2Te_4/(Bi_2Te_3)_n$
8	2020-10-27	李　毅 Yi Li	沈阳材料科学国家中心材料动力学研究部 Shenyang National Laboratory for Materials Science, Institute of metal research, Chinese Academy of Sciences, China	缺口对非晶机械性能的影响
9	2020-10-28	薛晓峰 Xiao-Feng Xue	北京交通大学 Beijing Jiaotong University	A brief survey of contact processes

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
10	2020-11-6	冯　波 Bo Feng	浙江大学 Zhejiang University	Expansion of EYM Amplitudes in Gauge Invariant Vector Space
11	2020-11-7	金　石 Shi Jin	上海交通大学 Shanghai Jiao Tong University	Semiclassical computational methods for quantum dynamics with band-crossing and uncertainty
12	2020-11-10	仲杏慧 Xing-Hui Zhong	浙江大学 Zhejiang University	Energy-Conserving Discontinuous Galerkin Methods for Vlasov Systems
13	2020-11-12	汪　涛 Tao Wang	重庆大学 Chongqing University	Floquet Engineering on Sr-87 optical lattice clock system
14	2020-11-12	成　娟 Juan Cheng	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	High order positivity-preserving and conservative DG schemes for radiation transfer equations
15	2020-11-16	朱天琪 Tian-Qi Zhu	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	Bayesian selection of misspecified models is overconfident and may cause spurious posterior probabilities for phylogenetic trees
16	2020-11-17	许现民 Xian-Min Xu	中国科学院数学与系统科学研究院 Institute of Computational Mathematics, Chinese Academy of Science	Model reduction methods for two-phase flows based on the Onsager variational principle
17	2020-11-17	周珍楠 Zhen-Nan Zhou	北京大学 Peking University	Fokker-Planck equations of neuron networks: rigorous justification and numerical simulation
18	2020-11-17	李会元 Hui-Yuan Li	中国科学院软件研究所 Institute of Software Chinese Academy of Sciences	Fourier Analysis and Laplacian Eigenvalues on Some Tetrahedra
19	2020-11-19	张　磊 Lei Zhang	北京大学北京国际数学研究中心 Beijing International Center for Mathematical Research, Peking University	构建能量景观上的解景观
20	2020-11-23	王　雷 Lei Wang	华北电力大学（北京） North China Electric Power University	高维转换波及其机制
21	2020-11-23	许　韬 Tao Xu	中国石油大学（北京） China University of Petroleum, Beijing	Rational solutions of the defocusing nonlocal nonlinear Schrödinger equation: Asymptotic analysis and soliton interactions

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序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
22	2020-11-25	贾伟乐 Wei-Le Jia	中国科学院计算技术研究所 Institute of Computing Technology, Chinese Academy of Sciences	HPC + AI + 物理模型：智能超算应用的新发展
23	2020-11-26	李铁军 Tie-Jun Li	北京大学 Peking University	Dynamical Approaches in scRNA-seq Data Analysis
24	2020-11-27	赖秀兰 Xiu-Lan Lai	中国人民大学 Renmin University of China	Modeling of axonal organelle accumulation induced by reduction of molecular motors
25	2020-11-27	于海军 Hai-Jun Yu	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	Learning Stable and Interpretable Low-dimensional Dynamics using Neural Networks with Rectified Quadratic Units
26	2020-11-28	王灯山 Deng-Shan Wang	北京师范大学 Beijing Normal University	Asymptotic analysis of the focusing NLS equation and focusing KE equation
27	2020-11-30	胡煜成 Yu-Cheng Hu	首都师范大学 Capital Normal University	Biological Image Analysis: Algorithm, Modeling and Simulation
28	2020-12-2	李　琼 Qiong Li	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	化学自由能模型改进及其在氢同位素的宽区域物态方程研制中的应用
29	2020-12-3	胡　俊 Jun Hu	北京大学 Peking University	A family of mixed finite elements for the biharmonic equations on triangular and tetrahedral grids
30	2020-12-3	刘文军 Wen-Jun Liu	北京邮电大学 Beijing University of Posts and Telecommunications	光孤子理论及其实验研究
31	2020-12-8	黄秋梅 Qiu-Mei Huang	北京工业大学 Beijing University of Technolgy	Discontinuous Galerkin methods for delay differential equations
32	2020-12-8	朱华星 Hua-Xing Zhu	浙江大学 Zhejiang University	Double-slit interference at the LHC using jet substructure
33	2020-12-10	张　亮 Liang Zhang	苏州大学 Soochow University	原位同步辐射X射线谱学技术在能源材料的应用

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
34	2020-12-15	Hailong Guo	墨尔本大学 University of Melbourne	Parametric polynomial preserving recovery
35	2020-12-22	舒其望 Chi-Wang Shu	布朗大学 Brown University	Stability of time discretizations for semi-discrete high order schemes for time-dependent PDEs
36	2020-12-22	张振宇 Zhenyu Zhang	中国科学技术大学 University of Science and Technology of China	Predictive Discoveries of 2D Materials for Topological Superconductivity and High-Tc Superconductivity
37	2021-1-5	王立联 Li-Lian Wang	新加坡南洋理工大学 Nanyang Technological University	A Truly Exact Perfect Absorbing Layer for Time-Harmonic Wave Scattering Problems
38	2021-1-8	郭秋江 Qiu-Jiang Guo	浙江大学物理系 Department of Physics, Zhejiang University	Probing Many-Body Physics with Superconducting Qubits
39	2021-1-11	王成 Cheng Wang	美国麻省大学达特茅斯分校 University of Massachusetts Dartmouth (UMassD)	Optimal rate convergence analysis and error estimate of a finite difference scheme for the Ericksen-Leslie system with the penalty function
40	2021-1-15	孙麓岩 Lu-Yan Sun	清华大学 Tsinghua University	基于玻色模式的量子信息处理
41	2021-1-18	李步扬 Bu-Yang Li	香港理工大学 The Hong Kong Polytechnic University	A bounded numerical solution with a small mesh size implies existence of a smooth solution to the Navier–Stokes equations
42	2021-1-25	邹青松 Qing-Song Zou	中山大学 Sun Yat-sen University	A preliminary study of the theoretic analysis of the spectral volume method for hyperbolic equations
43	2021-1-25	陈文斌 Wen-Bin Chen	复旦大学 Fudan University	Some numerical schemes for the Stokes-Darcy and the Cahn-Hilliard-Stokes-Darcy system
44	2021-2-5	徐　昆 Kun Xu	香港科技大学 The Hong Kong University of Science and Technology	统一气体动理学格式的发展和展望
45	2021-2-22	徐　岩 Yan Xu	中国科学技术大学 University of Science and Technology of China	Higher order accurate bounds preserving time-implicit discretizations for the nonlinear time-dependent equations

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46	2021-3-1	Bo Li	美国加州大学圣地亚哥分校 University of California, San Diego	Prediction of Molecular Binding/ Unbidning with Impilcit Solvent: Geometrical Flow, Transition Paths, and Brownian Dynamics
47	2021-3-2	张志跃 Zhi-Yue Zhang	南京师范大学 Nanjing Normal University	Numerical Methods for Parabolic Optimal Control Problem
48	2021-3-8	Lin Mu	美国乔治亚大学 University of Georgia	Pressure Robust Scheme for Incompressible Flow
49	2021-3-12	Jingwei Hu	美国普渡大学 Purdue University	A new stability and convergence proof of the Fourier-Galerkin spectral method for the spatially homogeneous Boltzmann equation
50	2021-3-12	Zhenning Cai	新加坡国立大学 National University of Singapore	On the method of complex Langevin
51	2021-3-22	赵　山 Shan Zhao	美国阿拉巴马大学 Department of Mathematics, University of Alabama	On solving elliptic interface problems with fourth order accuracy and FFT efficiency
52	2021-3-24	王　涵 Han Wang	北京应用物理与计算数学研究所 Institute of Applied Physics and Computational Mathematics	Modeling the interatomic potential by deep learning
53	2021-3-29	向淑晃 Shu-Huang Xiang	中南大学 Central South University	Approximation based on orthogonal polynomials and their roots
54	2021-3-31	邵嗣烘 Si-Hong Shao	北京大学数学科学学院 School of Mathematical Sciences, Peking University	Computational Quantum Mechanics in Phase Space
55	2021-4-1	王雨顺 Yu-Shun Wang	南京师范大学 Nanjing Normal University	哈密尔顿系统一类带自由参数的高阶保结构算法
56	2021-4-1	李凤艳 Feng-Yan Li	美国伦斯勒理工大学 Rensselaer Polytechnic Institute (RPI)	Asymptotic-preserving IMEX-DG methods for a linear kinetic transport model: different reformulations and IMEX strategies

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
57	2021-4-9	陈　鸿 Hong Chen	同济大学 Tongji University	非厄密量子原理启发的无线电能传输变革性技术
58	2021-4-12	许志强 Zhi-Qiang Xu	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	相位恢复: 理论、模型与算法
59	2021-4-12	张林波 Lin-Bo Zhang	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	数值积分与有限元计算
60	2021-4-13	王冬岭 Dong-Ling Wang	西北大学 Northwest University	Complete monotonicity-preserving numerical methods for time fractional ODEs
61	2021-4-16	刘　浩 Hao Liu	湖南大学 Hunan University	温稠密氢对电子阻止本领的电子力场方法模拟研究
62	2021-4-16	张　珅 Shen Zhang	国防科技大学 National University of Defense Technology	温/热稠密物质状态方程和输运性质的第一性原理研究
63	2021-4-20	梅立泉 Li-Quan Mei	西安交通大学 Xi'an Jiaotong University	等离子体物理中数学问题及其数值求解
64	2021-4-22	张　元 Yuan Zhang	郑州大学 Zhengzhou University	金属纳米腔增强单分子共振拉曼散射的非线性效应
65	2021-4-23	陈楚楚 Chuchu Chen	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	Accelerated Exponential Euler Scheme for Stochastic Heat Equation: Convergence Rate of Densities
66	2021-4-23	徐　劼 Jie Xu	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	Towards macroscopic liquid-crystal theory for general rigid molecules
67	2021-4-24	孙博文 Bo-Wen Sun	同仁医院 Tongren Hospital, China	视神经损伤临床科普

CSRC SEMINAR 专题报告

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
68	2021-4-24	代从新 Cong-Xin Dai	同仁医院 Tongren Hospital, China	图像识别在神经外科领域的应用
69	2021-4-26	孙伟伟 Weiwei Sun	北京师范大学-香港浸会大学联合国际学院 BNU-HKBU United International College	Numerical Methods and Analysis for Landau-Lifshitz equation
70	2021-4-27	樊玉伟 Yu-Wei Fan	华为公司中央研究院理论研究部 Huawei theory Academia Sinica Research Department, China	工程应用中的几个计算数学小问题
71	2021-4-27	谢小平 Xiaoping Xie	四川大学 Sichuan University	Discontinuous Galerkin method for a distributed optimal control problem of time fractional diffusion equation
72	2021-4-28	季　霞 Xia Ji	北京理工大学 Beijing Institute of Technology	Inverse scattering with multi-frequency sparse data
73	2021-4-28	邓明华 Ming-Hua Deng	北京大学 Peking University	基于深度学习的单细胞聚类与标注
74	2021-4-29	沈晓芹 Xiao-Qin Shen	西安理工大学 Xi'an University of Technology	Steady and unsteady flexural shell models and numerical computation
75	2021-4-29	周天寿 Tian-Shou Zhou	中山大学 Sun Yat-Sen University	基因表达调控系统的建模与分析
76	2021-5-6	张　磊 Lei Zhang	北京大学 Peking University	Deciphering Embryonic Morphogenesis with a Data-driven Phase Field Model
77	2021-5-7	邱蔚峰 Weifeng Qiu	香港城市大学 City University of Hong Kong	On a discrete embedding inequality for two types of fourth order elliptic equations (Biharmonic and Quad-Curl)
78	2021-5-10	李　舟 Zhou Li	中国科学院空天信息研究院粤港澳大湾区研究院 GBA Research Institute of AIRCAS	太赫兹基础科学研究——从电声子相互作用谈起

序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
79	2021-5-13	项　阳 Yang Xiang	香港科技大学 Hong Kong University of Science and Technology	Modeling and Simulation for Dislocation Climb
80	2021-5-13	明平兵 Ping-Bing Ming	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	A Nitsche type Multiscale Method with Non-matching Grids
81	2021-5-14	石　猛 Meng Shi	中国科学院空间应用工程与技术中心 Technology and Engineering Center for Space Utilization, CAS	原子自旋陀螺仪工作原理及应用
82	2021-5-18	包承龙 Cheng-Long Bao	丘成桐数学科学中心 Yau Mathematical Sciences Center	Robust Modeling In Image Processing
83	2021-5-18	王家赠 Jiazeng Wang	北京工商大学 Beijing Technology and Business University	Voltage Responses to the Channel Noise: The Power Spectrum
84	2021-5-20	翟起龙 Qi-Long Zhai	吉林大学数学学院 School of Mathematics, Jilin University	Schrödinger方程的深度学习方法
85	2021-5-24	凤小兵 Xiaobing Feng	美国田纳西大学诺克斯维尔分校 University of Tennessee, Knoxville	Fully Nonlinear Second Order PDEs and Their Numerical Solutions
86	2021-5-27	彭智慧 Zhi-Hui Peng	湖南师范大学 Hunan Normal University	基于超导量子电路的混合系统研究
87	2021-5-28	魏凤英 Fengying Wei	福州大学 Fuzhou University	Monte Carlo Simulations of SDE Competition Models
88	2021-5-28	谢和虎 He-Hu Xie	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	扩展子空间算法及其应用
89	2021-5-31	张　原 Yuan Zhang	北京大学 Peking University	On Geometries of Finitary Random Interlacements

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序号	DATE\日期	SPEAKER\报告人	INSITUTE\单位	TITLE/报告题目
90	2021-6-2	Cheng Wang	美国麻省大学达特茅斯分校 University of Massachusetts Dartmouth	Structure-preserving, energy stable numerical schemes for a liquid thin film coarsening model
91	2021-6-3	张世华 Shi-Hua Zhang	中国科学院数学与系统科学研究院 Academy of Mathematics and Systems Science, CAS	深度学习的数学理解
92	2021-6-3	蒋仲庆 Zhong-Qing Jiang	浙江理工大学 Zhejiang Sci-Tech University	碳基氧功能电催化材料及能源器件应用
93	2021-6-11	董兆楠 Zhao-Nan Dong	法国国家数字科学技术研究所 National Institute for Research in Digital Science and Technology	A posteriori error analysis for discontinuous Galerkin methods on polygonal and polyhedral meshes
94	2021-6-22	廖洁桥 Jie-Qiao Liao	湖南师范大学 Hunan Normal University	腔光力系统中多个力学模式的协同基态冷却
95	2021-6-24	周栋焯 Douglas Zhou	上海交通大学 Shanghai Jiao Tong University	单个神经元与神经元网络的建模
96	2021-6-29	李逸飞 Yi-Fei Li	新加坡国立大学 National University of Singapore	An energy-stable parametric finite element method for anisotropic surface diffusion
97	2021-7-14	Abolfazl Bayat	电子科技大学 University of Electronic Science and Technology of China	Quantum Simulation in NISQ Era
98	2021-7-23	杨志国 Zhiguo Yang	上海交通大学 Shanghai Jiao Tong University	The gPAV method for devising efficient and stable schemes for multi-phase flow systems

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COLLOQUIUMS 百旺科学论坛

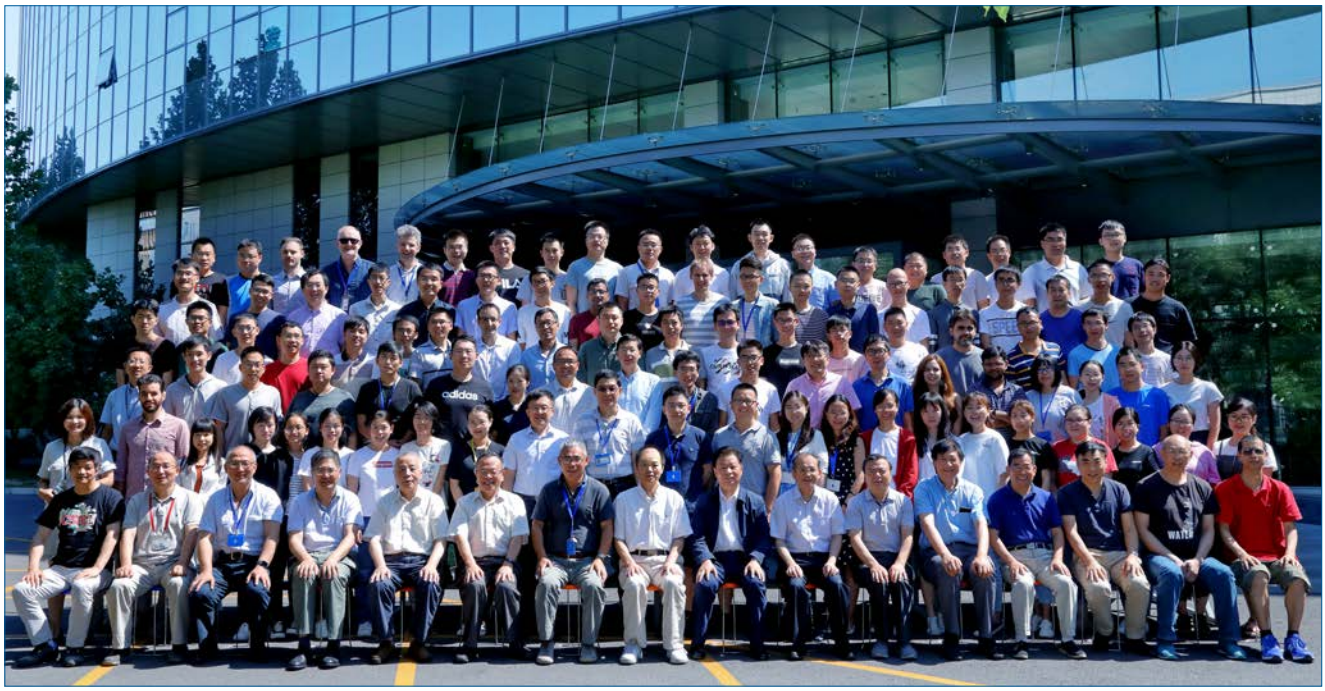
百旺科学论坛是由中物院研究生院、北京计算科学研究中心、北京高压科学研究中心联合举办的高端学术论坛。论坛组织邀请国内外优秀学者做前沿科学报告。论坛侧重于基础科学研究，致力于为广大科研工作者提供不同的视角，提供展示交流的平台，促进学科交叉相互启发，对重要的科学进展进行普及。自开展至今已举办四期。

To facilitate scientific interactions between CSRC scientists and scientists elsewhere, CSRC has developed partnerships with several universities and research institutions around the world. Besides engaging in long-term scientific collaborations, CSRC staff also host conferences, workshops, and seminars with collaborators. Through these activities, CSRC is working towards extending the frontier in computational science research and improving its competitive edge and prestige.

北京计算科学研究中心非常重视与科研机构及高校的合作，在积极组织承办国内外学术会议之时，也鼓励科研人员与国内外其他科研机构之间的互访交流，扩展学术视野和扩大学术影响。目前已与国际数所科研机构签署了合作协议，为打造中心作为国际一流的开展计算科学及相关学科交叉研究的综合平台而不断努力。

INTERNATIONAL PARTNERSHIP 国际及地区合作伙伴

- UNIVERSITY OF GOTHENBURG, SWEDEN 瑞典哥德堡大学
- UNIVERSITY OF OSLO, NORWAY 挪威奥斯陆大学
- INSTITUTE FOR QUANTUM COMPUTING, UNIVERSITY OF WATERLOO, CANADA 加拿大滑铁卢大学
- NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY, NORWAY 法国原子能与可替代能源委员会
- UNIVERSITY OF WARWICK, UK 英国华威大学
- CENTER FOR SIMULATIONAL PHYSICS, THE UNIVERSITY OF GEORGIA, USA 美国乔治亚大学
- NTNU NORWEGIAN UNIVERSITY OF SCIENCE AND TECHNOLOGY, NORWAY 挪威科技大学
- THE HONG KONG UNIVERSITY OF SCIENCE AND TECHNOLOGY, CHINA 香港科技大学
- COLLEGE OF SCIENCES, OLD DOMINION UNIVERSITY, USA 美国奥多明尼昂大学
- RIKAGAKU KENKYUSHO/INSTITUTE OF PHYSICAL AND CHEMICAL RESEARCH, JAPAN 日本理化学研究所
- DEPARTMENT OF PHYSICS, NATIONAL TAIWAN NORMAL UNIVERSITY, CHINA 国立台湾师范大学
- DEPARTMENT OF PHYSICS, THE CHINESE UNIVERSITY OF HONG KONG, CHINA 香港中文大学
- HEARNE INSTITUTE FOR THEORETICAL PHYSICS, LOUISIANA STATE UNIVERSITY, USA 美国路易斯安那州立大学
- KOREA INSTITUTE FOR ADVANCED STUDY, SOUTH KOREA 韩国高等科学院



Since its establishment, more than 5000 visiting scholars from over 20 countries and regions have visited CSRC. CSRC faculty members went out for academic eschange for more than 2000 times. During the academic year 2020-2021, CSRC has hosted over 200 visiting scholars.
CSRC warmly welcomes scientists around the world to visit for collaboration and exchange. CSRC frequently hosts academic activities such as conferences, workshops, and seminars together with its counterparts. Living allowance and housing subsidies are provided during visitor's stay at CSRC.

中心在加强与科研机构及高校的合作交流，积极组织承办国内外学术会议之余，也鼓励科研人员与国内外其他科研机构之间的互访交流。成立至今，中心接待了来自20多个国家和地区的访问学者超过5000余人次，中心科研人员外出参加学术交流活动超过2000余人次。2020-2021学术年期间，中心来访学者超过了200人次；受因疫情影响，访问交流逐渐向线上等多元化模式发展。

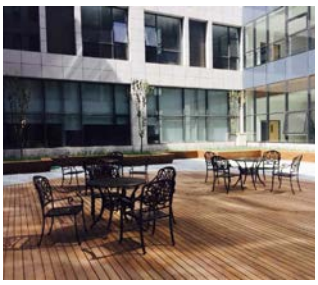
中心欢迎国内外各机构相关专业的科研人员和教师，以访问学者和客座研究人员的形式来访，进行短期或长期合作研究。中心也与同行们一起举办学术活动如会议、讲习班等。在中心访问期间，中心将提供一定的生活和住房补贴。

〖 中心办公楼效果图 〗 CSRC building

〖 中关村软件园一二期鸟瞰图 〗 ZPark

〖 大厅 〗 Lobby

〖 中庭院 〗 Courtyard

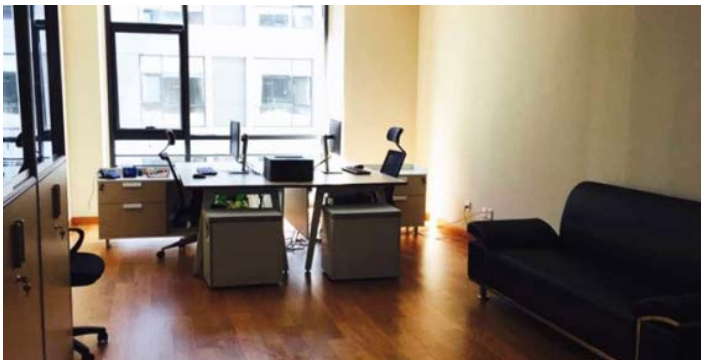


〖 学术报告厅 〗 Auditorium

Seminar Rom 〖 学术会议室 〗

Common 〖 学术讨论区 〗

〖 博士后办公室 〗 Postdoc Office



Visitor Office 〖 客座教授办公室 〗

〖 访问学者办公室 〗 Visitor Office

〖 健身房 〗 Gym

〖 餐厅 〗 Canteen

天河二号-计科中心集群系统
CLUSTER TIANHE2-JK

The CSRC is equipped with the state of art high performance computing facilities, which include a dedicated in-house 14,000+ core cluster TianHe2-JK in addition to many smaller clusters.

For more details about CSRC Computing, please visit: http://www.csrc.ac.cn/en/facility/cmpt/

14112cores

131.1TB Memory

1440TB disks
2304TB back-up disks

80Gb/s QDR